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Screening level estimation of release rates of currently used chemicals to the environment – application to solution-oriented assessment of impacts on aquatic ecosystems

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Dissemination Level		
PU	Public	
PP	Restricted to other programme participants (including EC)	
RE	Restricted to a group specified by the consortium (including EC)	
CO	Confidential, only for members of the consortium (including EC)	

1.1 Summary

This Deliverable presents the basis for, approach to and results of the SOLUTIONS team efforts on emission estimation of chemicals on the European scale. The task in the context of the SOLUTIONS project was, to provide a generic emission model for all chemicals on the European market, that can be applied on the European scale, operating on realistic numbers of types of available data, and that feeds into further assessment steps. It is explicitly noted, that environmental assessment models can start from two opposing principles, viz. a start from single chemicals to build the case of European-scale chemical exposures, risks and impacts by continuous addition of chemicals to the assessment, or a start from the viewpoint that screening-level results can be obtained when building the case from available data on very many chemicals with lower precision per chemical. This Deliverable started from the latter perspective, and was aimed to deliver screening-level insights into emissions of chemicals at the European scale. Those were further applied in detailed analyses of exposure levels and associated risks and impacts, based on modelling with an integrated chemical-hydrological-(eco)toxicological "model train". Data analyses with the integrated model train, providing the more refined insights into geospatially explicit concentrations and impact estimates for human health and the environment, based on geospatially explicit use of the emission model. Those provide the opportunity to derive refined (spatiotemporally specific) insights into risks of chemicals and their mixtures. Both the screening-level and the refined outputs eventually provide relevant information for water quality protection, assessment and management.

The present approach describes the analyses of a screening-level emission model, and the results of a first-tier assessment of prioritization of chemicals. The approach is based on production data and practically applied approaches to quantify emissions. The resulting model is a generic emission model for all compounds on the European market. By virtue of the principles prescribed for its derivation, the

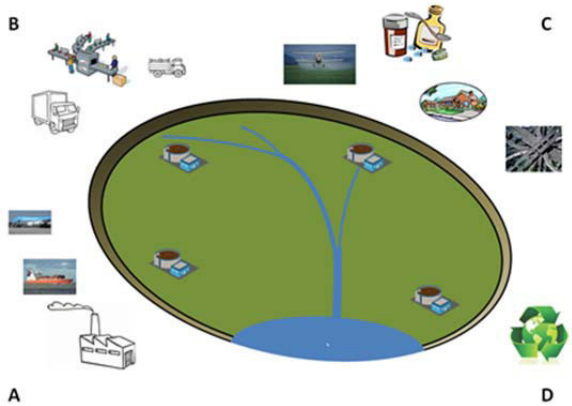
model is aimed to serve screening purposes, that is: to discriminate between groups of chemicals, in this case at the level of their potential to cause harm. That approach to prioritization expands on approaches that consider e.g. emission potentials or hazard characteristics only.

Similar to other studies on screening-level approaches, this study clearly shows that screening-level emission assessments can discriminate between chemicals groups, in this case: those that likely pose no harm and those that might, at the studied scale. It is noted that the screening-level assessment is closely associated to the available data and models used in regulatory chemical risk assessments.

One of the key aspects of emission estimation on the European scale is that the model outcomes cannot be directly validated, or in other words: validation requires comparison of predicted and observed concentrations in European water systems, so a comparison involving data that are obtained after the subsequent step of fate modelling. Hence, validation information was obtained by comparing the outcomes of the SOLUTIONS model train, and these comparisons were produced by SOLUTIONS-partner Deltares and reported in Deliverable D14.2 (in prep.).

The Deliverable encompasses the text for a publication in the open literature, representing data for more than 6000 compounds. The Deliverable includes the Supporting Information on those compounds, allowing for further use of these data for various purposes in environmental protection, assessment and management. The text will be finalized and submitted for publication when the required results of the SOLUTIONS model train over-all validation have been finalized and adopted, and will then be published together with a twin-paper that supports the risk assessment of the studied compounds and their mixtures in surface water bodies.

1.2 [publishable] Graph



Releases of chemical substances are estimated for a variety of uses of chemicals in all life cycle stages: manufacturing and transport (A), formulation and distribution (B), service life (C) and recycling/waste

stage (D). In most uses, release to the environment takes place after waste water treatment. This Deliverable considers European production volumes and emission rates of many chemicals, as basis for spatio-temporally explicit predictions of chemical concentrations and mixture risks in European waters.

2. List of Contents

The contents of the Deliverable consist of:

a. The text of a publication on emission estimation
b. Supporting Information, in a format allowing for use in the SOLUTIONS-model train, for 6416 identified substances

Note that the Supporting Information also encompasses the information collected for the studied compounds related to modelling the toxic pressure of the studied chemicals, as resulting from the work of the SOLUTIONS Modeller's team (WP18), which allows for utilizing these data for environmental protection, assessment and management beyond the SOLUTIONS project.

3. List of Abbreviations

See publication text.

Screening level estimation of release rates of currently used chemicals to the environment – application to solution-oriented assessment of impacts on aquatic ecosystems

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ABSTRACT

Aims and context. In support of solution-focused integrated modeling of the risks of chemicals in the context of water quality protection, assessment and management in the EU-SOLUTIONS project, this paper describes a novel method to estimate environmental release rates of all chemical substances currently used in Europe. Rather than starting from detailed per-chemical approaches, a generic screening-level approach was developed, closely related to and building forth on the regulatory assessment of chemicals in the European Union. This explicitly encompasses the ambition of the EU-SOLUTIONS project to consider all chemicals currently in use, as well as to enable considering emerging chemicals.

Approach. The generic screening approach was developed using relatively simple but available data. It consists of collecting European-wide production masses of chemicals, followed by screening-level generic assessment of emitted fractions, utilizing Environmental Release Category data. The novel emission estimation method has been applied to and tested for plausibility and functionality on chemicals registered until April 2015 under the EU chemicals regulation REACH, active ingredients of medicines registered under the EU medicine regulation and active ingredients of crop protection products registered under the EU pesticide regulation.

Results. The emission estimation method, combined with the SOLUTIONS-model train approach to predict local ambient concentrations, yielded showed that the net predicted concentrations associated reasonably well to measured concentrations for chemicals for which field data were obtained. The predicted emissions were further utilized in a screening-assessment involving assessment of the mixture toxic pressure of a typical EU-water body, as defined to execute a regulatory chemical assessment. The mixture toxic pressure for a typical 'EU-water' in steady state conditions were in fair agreement to other (published) data on mixture toxic pressures based on both predicted and measured surface water concentrations of chemicals. The screening results further resulted in a clear prioritization pattern, in which 95% of the predicted mixture effects caused by direct impacts on species vital traits can be attributed to a top-5% of chemicals at the selected (large) scale. This is a finding also found with other screening-level or refined emission, exposure or impact assessments, and it is valuable for prioritization of management attention and efforts.

Interpretation and relevance. The results of the present study are interpreted as a screening-level opportunity in chemical assessment and management that involves "excluding the innocent", here amounting to grossly 95% of the compounds investigated. This boils down to a non-prioritization of

these compounds for management, given the dominance of 5% of the studied chemicals in potentially causing direct toxicological impacts at the European scale. We note that similar studies would be required for other exposure pathways, such as secondary poisoning, to similarly evaluate non-prioritization for chemicals exerting toxicity via that pathway too. This interpretation is a logically solid, but screening-level basis to prioritize management of harmful substances, as subsets of chemicals that are excluded and included for management are vastly different in their potential to cause harm by direct exposure on the scale of the EU. Within the group of ¬ 5% chemicals of concern, uncertainties in the emission, fate and effect modeling imply that a strict priority rank order of risks posed by individual chemicals in this subset cannot be derived from the available European data, and we argue that this is also unnecessary. This group can, however, be subjected to a next tier of (spatially explicit) evaluation, with integrated SOLUTIONS-based models, as described elsewhere. Note that a regulatory choice other than the 95-5 distinction can be made, whereby more conservative approaches (e.g., 90-10) can be chosen.

Conclusions. We conclude that the emission rates of chemicals used in Europe can be estimated with sufficient accuracy and precision to allow assessment of expected impacts of their use on aquatic ecosystems in a way useful for a screening-level in the context of chemical and environmental risk assessment and management. We emphasize that the approach presented in the present study is in line with the holistic nature of the EU Water Framework Directive, which has been built on system-level principles. That is, the current study provides a screening-level and systems-oriented approach to sub-select chemicals for management on the European scale related to emissions and expected impacts, which can be followed by a site- and substance oriented approach in chemical management. The SOLUTIONS model train support creating a refined, spatio-temporally explicit assessment of expected exposures and mixture risks, expanding on the screening-level assessment presented in the present paper. The screening-level prioritization resulting from the generic assessments presented may support an efficient use of the refined assessment approach, but evaluating the potentially most-relevant chemicals with priority.

INTRODUCTION

This study was done as part of the EU FP7 project 'SOLUTIONS' (Brack et al., 2015), in which tools and models for environmental decision making are developed. Among other things, the SOLUTIONS project develops descriptive and predictive models to simulate impacts of toxic substances and their mixtures in aquatic ecosystems, in relation to chemical-, soil- and water management. The ambition of the SOLUTIONS project is, to collect data on all chemicals currently in use in Europe, and to investigate their production, emission, ambient concentrations and (mixture) impacts, in order to support environmental protection, assessment and management. Hence, the present paper aimed to provide a generic approach relevant for all chemicals (currently used, and emerging chemicals), which can operate on relatively few (available) data, and that provides screening-level but relevant results for water quality management purposes. Other approaches, amongst others in the SOLUTIONS-project, aimed to provide spatio-temporally explicit exposure and impact information for the same uses. Both approaches, screening-level and refined, can eventually serve in a tiered scheme, whereby the former supports selection of the chemicals relevant for the latter, more data-intensive, analyses.

The starting point for modeling impacts of chemical substances is knowledge of the amounts of chemicals that are released (intentionally or unintentionally) to the environment as a consequence of production and use downstream in the production-use-waste chain. Emitted mass, combined with characteristics of the environment (e.g., the volume of environmental compartments), result in exposure concentrations, and combining those with knowledge on toxicities of individual chemicals, allows for quantifying impacts of chemicals, alone or in mixtures. A companion paper on hazard information of chemicals provides the latter information[1].

Contemporary models that are used to describe and predict exposure concentrations assume first-order kinetics (Cowan et al., 1995; McLeod et al., 2008) and are linear with respect release rates: predicted environmental concentrations are directly proportional to the emission rates and are thus used as input to the further exposure and impact calculations. Uncertainty in emission rates translates directly into uncertainty in modeled concentrations. The first challenge in estimating release rates for the SOLUTIONS project – the subject of the present paper – is to obtain sufficient accuracy and precision to allow sufficiently accurate and precise exposure- and impact modeling of all chemicals produced and emitted due to human activities. The second challenge is to identify those chemicals – from > 100,000 currently produced and used – that likely significantly contribute to environmental impacts, and discriminate those that are unlikely to do so. Enabling a judgment of those chemicals that unlikely pose harm from those that might is considered of high practical value, as it is expected that this might help focus on relevant chemicals rather than on all. Since it is as yet unknown which chemicals do and which

[1] This paper is currently in prep.; it builds on SOLUTIONS product ID M5.2, and currently contains more than 12,000 Species Sensitivity Distribution models. It is in the Reference list as "SOLUTIONS-WP18 (In prep.). Chemicals and their potential to cause ecological harm. Supporting environmental assessment and management via Species Sensitivity Distribution modeling for >12,000 chemicals."

chemicals do not contribute significantly, environmental decision makers currently have no other option than to consider all chemicals as potentially significant, whilst there is nearly no knowledge regarding the net probable effects of all chemicals released.

Given the current needs in water quality protection, assessment and management regarding chemicals, and in view of the prioritization needs, release rates of all chemicals that are currently used were estimated, and exposure- and impact assessments were made for as many chemicals as feasible, i.e., 6416, as determined by data availability. The number of currently used chemicals is large and increasing (Bernhardt et al., 2017). At the start of the SOLUTIONS project in 2013, more than 10,000 individual chemical substances had been registered under the EU chemicals' regulation REACH (https://echa.europa.eu/information-on-chemicals). Many more compounds are still being offered for registration and new chemicals are continuously being developed. Further, thousands of active ingredients for medicines and crop protection products have been registered and are being registered. For a comprehensive approach to water quality protection, assessment and management, it is required to make a comprehensive effort on estimating release rates, exposure concentrations and potential impacts of all these chemicals, and to quantify their expected (combined) exposure and mixture impacts on aquatic ecosystems. The SOLUTIONS-project aimed to follow such a comprehensive approach, and the present paper concerns the aspect of emission estimation with that effort; other steps on the pathway from emission to impacts are subject of related studies published elsewhere[2].

We have developed an estimation procedure capable of delivering the release rates necessary for comprehensive impact assessments of chemical produced and used in Europe, with a practice-oriented approach. That is, the method was designed to be applicable in general, for compounds as developed and produced for which it is acknowledged that commonly minimal data types and numbers are available. We have applied this method to all chemical substances that are known to be used at present in Europe and for which such data could be obtained. We have tested the resulting release rates for plausibility and functionality by comparing predicted and observed concentrations for chemicals for which the latter data were available[3], and by making screening-level impact assessments of expected concentrations in so-called 'EU water', i.e. imaginary fresh water (ECHA, 2016) as modeled in REACH to demonstrate the possibility to use chemicals 'safely', as required for registration under REACH.

The aims of the present paper are to (1) describe the emission estimation approach that was developed to estimate emission rates for a vast number of chemicals, based on relatively minimal data, (2) describe the accuracy of the outcomes of this model by comparing predicted and observed concentrations of substances for which the latter data were available, and (3) to compare the predicted mixture toxic pressure, and the contributions of the individual chemicals to that for the regional EU-water, to provide a screening-level discrimination of chemicals which are of higher and lesser importance for management

[2] Currently, the most relevant companion studies are prepared as SOLUTIONS-Deliverable D14.2 (in prep.) and the risk assessment models developed and utilized in SOLUTIONS WP18, regarding human health and environmental risk assessments, for separate species and species assemblages respectively.
[3] Utilizing results in D14.2 (in prep.)

on the European scale, based on the principles used for REACH, and (4) discuss the results in relation to the use of these outcomes in a tiered fashion, in which the present paper describes the screening-level evaluation of many chemicals, and associated papers a spatio-temporally explicit and refined approach to predicting exposure to and impacts of chemicals.

METHODS

A large variety and number of data were collected and used for modeling. The main text describes data sources and approaches, whilst the Supporting Information (various tables) contains details.

Collection of use volumes

Manufacturers of chemical substances report amounts produced and marketed to regulatory authorities as part of the obligatory submission of pre-registration information. The information that is submitted is generally strictly confidential, to be used only for registration purposes (e.g., https://echa.europa.eu/legal-notice). The SOLUTIONS project has obtained so-called 'EU tonnages' $EUtonnage = Production + Imports - Exports$ registration dossier data for the purpose of EU-wide analysis of environmental impacts of all chemical substances on the EU market from various sources.

REACH substances. EU tonnages of REACH-registered chemicals were provided by the European Chemicals Agency ECHA at request of the Netherlands Competent REACH Authority. EU tonnages of nearly 13,000 individual chemical substances, registered until April 2015 were made available for the present study (RIVM, 2015).

Active ingredients of medicines. Amounts of more than 1,000 individual pharmaceuticals sold in Sweden and the UK were obtained from public sources (Rahmberg, 2015; Boxall et al., 2015). Additional sales data for a lesser numbers of pharmaceuticals, sold in Austria, Switzerland, Germany, France and the Netherlands, were obtained from various other public reports (IKSR, 2009; Fent, 2006; Van der Aa, 2008, 2011).

Active ingredients of crop protection products. Amounts of active ingredients of crop protection products are monitored by individual EU member states and reported to the European Statistics Agency EUROSTAT. This agency combines the confidential original data into main categories of active ingredients. Original sales data of pesticides could not be made available for the present study. Instead, estimations made by the Joint Research Center of the European Commission by means of the so-called 'harvested area approach' (Sala et al, 2014, 2015) were used. Use volumes of over 400 active ingredients of crop protection products, used in different EU countries, were obtained.

Emission estimation

Different chemical groups have vastly different emission patterns. Some chemicals are made to be released to the environment. For instance, crop protection products used in open field applications are released almost entirely to crops and soils. Similarly, chemicals used in 'down-the-drain' household products easily find their ways into sewerage systems. Other chemicals are made for use as parts of durable products, from which very variable amounts are released into the environment. Yet other chemicals are not meant to be used as such at all, but serve as industrial intermediates, or as fuel in vehicles and power plants. We have developed a general-purpose substance-flow estimation procedure that accounts for these very different uses of chemicals with vastly different release rates.

The method is based on the generic A/B table method developed in the 1980s by Van der Poel and Ros (1995) for use in the European Union Substances Evaluation System EUSES, which is still in use as a method under REACH (ECHA, 2016). Releases of chemicals from all possible uses in the entire life cycle of chemicals are considered (Figure 1).

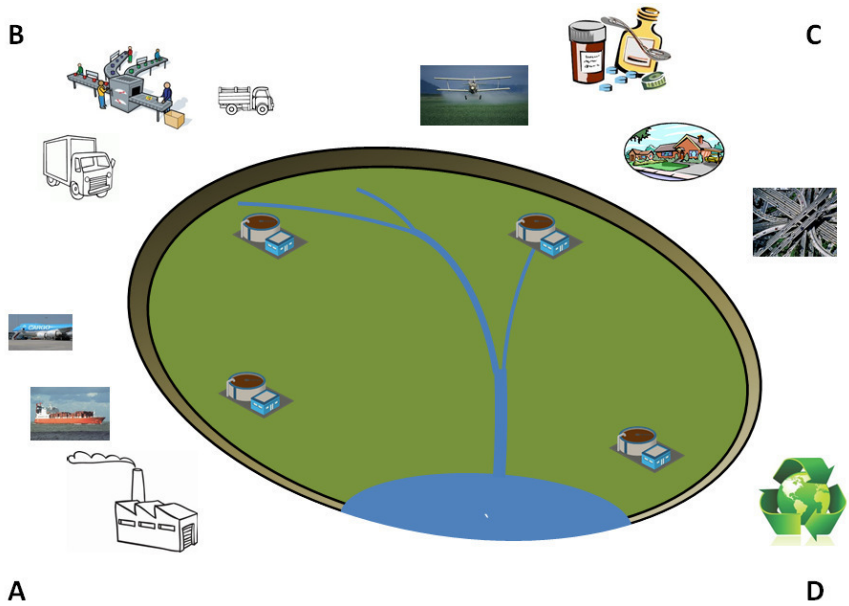

Figure 1. **Releases of chemical substances are estimated for a variety of uses in all life cycle stages: manufacturing and transport (A), formulation and distribution (B), service life (C) and recycling/waste stage (D). In most uses, release to the environment takes place after wastewater treatment.**

The generic approach discriminates various life stages and their generic characteristics:

Life cycle stage Ia. Small, but significant amounts of chemical may be released to air, (waste)water or soil directly from the first life cycle stage, during manufacturing or transport (Figure 1A), though exceptions with specific point-source releases may occur (e.g., Lindim et al., 2015). Manufacturing may or may not take place in Europe. Fractions of the overall tonnage, manufactured in Europe, are known from the REACH registration dossiers and are accounted for in emission estimation.

Life cycle stage Ib. Chemicals are rarely used without further processing. Generally, chemicals are formulated into products and distributed (Figure 1B) to other places in or outside Europe.

Life cycle stage II. During service life, chemicals are used in different ways and released to different degrees (Figure 1C). For most chemicals, the greatest releases take place during service life.

Life cycle stage III. Small but increasing fractions of chemicals produced and used are recycled (Figure 1D). In most life cycle stage uses, chemicals undergo treatment in wastewater treatment facilities, which usually retain most, but certainly not all of the chemicals.

When expressed as a mathematical formula, the emission estimation process reads:

$$E_{i,j,k} = \sum_{i,j,k}\left(UseVol_i \cdot ActCat_{i,j}\right) \cdot RF_{j,k} \cdot Fstp_{i,k}\ , \qquad (1)$$

where $E_{i,j,k}$ denotes the EU-wide emission rate of substance i from use j into environmental medium k, $UseVol_i$ [tpa] is the EU tonnage of chemical i, $ActCat_{i,j}$ is the fraction of the use volume of substance i, used in activity category j, $RF_{j,k}$ is the fraction [-] of this use that is released into medium k and $Fstp_{i,k}$ denotes the fraction of substance i released to medium k upon sewage treatment. Release fractions $RF_{j,k}$ are listed in Table 1.

Table 1. Estimated release fractions in the various uses and life cycle stages. Based on published and unpublished reports. (spERC = Specific Environmental Release Category)

Activity category		release	to air	to water	to soil
Stage I	Use1: MANUFACTURING [1]	0.4%	0.2%	95%	5%
Stage I	Use2: DISTRIBUTION & FORMULATION [1]	0.5%	60%	39%	1%
Stage I	Use3: INDUSTRIAL PROCESSING [1]	0.5%	59%	35%	6%
Stage II	Use4: USE in AGRICULTURE [2]	100%	15%	1%	84%
Stage II	Use5: USE in MEDICINE [3]	12%	0.0%	100%	0%
Stage II	Use6: WIDE-DISPERSIVE USE in 'down-the-drain' [1]	100%	0.0%	100%	0%
Stage II	Use7: Other WIDE-DISPERSIVE USES [1]	100%	73%	11%	16%
Stage II	Use8: WIDE-DISPERSIVE 'low-release' USES [1]	5%	73%	11%	16%
Stage II	Use9: USE as FUEL [4]	0.04%	96%	4%	0%
Stage II	Use10: Other stage-II USES [1]	0.5%	26%	22%	9%
Stage III	Use11: TREATMENT, RECYCLING [1]	5%	33%	33%	33%
Stage III	Use12: SOLID WASTE DISPOSAL [1]	10%	0.0%	0.0%	100%
Use-weighted averages, based on selected spERCs		25%	63%	31%	6%

[1] Cefic, 2012

[2] Sala et al., 2014, 2015

[3] IKBR, 2009; Fent et al., 2006; Van der Aa et al., 2008,2011

[4] Concawe, 2008

REACH substances. Fractions released to air, water and soil in specific uses in the different life cycle stages are aggregated from the 169 different uses for which industry has proposed standard values (Table SI-1, Supporting Information), claimed to be 'best possible estimates' (Cefic, 2012). Unfortunately, fractions of chemical used in the 169 spERC (specific Environmental Release Category) uses are not listed in REACH registration dossiers, and cannot be used to estimate emission rates with eq 1. At a screening level, use-volume weighted average release fractions are assumed for all REACH substances in all activity categories.

Pharmaceuticals. Pharmaceuticals are assumed to be used entirely according to Stage II, use 5 (use in medicine). Based on a publication by Lindim et al (2016), who studied releases of 56 pharmaceuticals in Sweden, we have assigned a release fraction of 12% of the human consumption rate, assumed to be released entirely to sewage treatment plants.

Crop protection products. Pesticides are assumed to be used entirely according to Stage II, use 4 (use in agriculture. Based on a study by Sala et al. (2014, 2015), who applied the so-called 'harvested area approach' to estimate releases to air, water, plants and soil, we assigned the release fractions listed in Table 1: 100% release to the environment (of which 15% to air, 1% to water and 84% to soil), without wastewater treatment.

EVALUATIONS

Validation of emission predictions of all chemicals in Europe through comparison to emission data is not feasible. Instead, two other approaches have been applied for the evaluation of the performance of the model and its outputs, focusing on exposure and impact metrics, respectively, namely:

(1) comparison of predicted and observed concentrations in European surface waters, which implies the comparison of observed concentrations with predicted concentrations which in turn result from the subsequent model steps of emission + fate modelling (Van Gils et al., in prep.)

and

(2) evaluation of predicted mixture toxic pressures resulting from emission estimation and known characteristics of the European water systems with other data on ambient aquatic mixture toxic pressures. The mixture toxic pressure metric is derived from quantifying the Potentially Affected Fraction (PAF) of species in a species assemblage from the (predicted or measured) ambient concentration of a chemical via Species Sensitivity Distribution (SSD) modelling (Posthuma et al., 2002). The mixture toxic pressure can subsequently be derived and expressed as msPAF (multi-substance PAF). In short, when the mixture toxic pressure for a series of water bodies has been determined, those can be ranked using their msPAF-values, with the interpretation that a higher rank associates to a higher probability that the mixture present in the water body poses harm to the species assemblage exposed in that water body (Posthuma and De Zwart, 206, 2012), including a limitation to maintain or reach Good or High Ecological Status (Posthuma et al., in prep.).

Both methods (comparing predicted to observed concentrations, and evaluation of mixture toxic pressure outcomes) were applied according to the approaches detailed below.

Evaluation 1 on exposures: predicted and observed concentrations

Predicted and observed concentrations assessments depended on the outcomes of the next step in the so-called SOLUTIONS model train, viz. fate modelling. These results were obtained by Van Gils et al. (in prep.), and the approaches and results are described in SOLUTIONS-Deliverable D14.2. The results of that assessment are summarized in the present paper.

Evaluation 2 on impacts: predicted mixture toxic pressures from the current and other studies

Since the conceptualization of mixture toxic pressures as a metric to rank ambient samples in their potential to cause harm to species assemblages, various studies have resulted in series of estimated values of the metric used, msPAF. These studies vary in composition (compound identities and exposure levels), and regarding measured and prediction concentrations. However, those form a basis to evaluate the expected ecotoxic impact outcomes related to the present screening-level emission estimates, given that those can be used according to current Guidance (ECHA, 2016) to predict chemical concentrations in typical (imaginary) 'EU water'. The latter approach requires some extra modelling steps, as explained below.

Evaluation 2 on impacts: approaches

Exposure estimation for typical EU-water body

Concentrations of chemicals in 'EU water', as expected on the basis of estimated emission rates were modeled using the 'SimpleBoxTreat' (Van de Meent et al., 2018). SimpleBoxTreat (Figure 2) is a simplified version of the combined environmental fate simulation models SimpleTreat (Struijs et al., 2016; Lautz et al., 2017) and SimpleBox (Hollander et al., 2016), developed for the German Federal Environment Office UBA, to be used in their decision support system KnowSEC (Striffler and Wassermann, 2015). The SimpleBoxTreat is set up to simulate steady-state concentrations in effluents and sludge from a generic sewage treatment plant, and in a generic receiving environment (air, water, soil) on local, regional and continental spatial scales. The physical and chemical substance properties required for modeling expected concentrations with SimpleBoxTreat were taken from the SOLUTIONS project's data compilation of the Modeler's List of Substances (Van Gils et al., 2018; Table SI-2, Supporting Information).

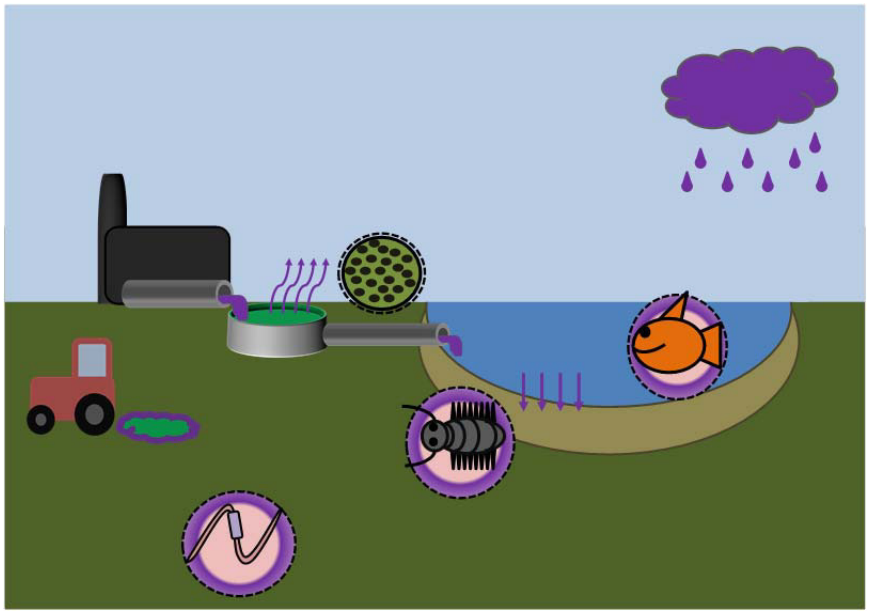

Figure 2. A simplified three-compartment version of the multimedia mass balance model SimpleBox (Hollander et al., 2016), combined with the sewage treatment plant simulation model SimpleTreat (Struijs et al., 2016), is used by the German Federal Environment Office (UBA) to calculate 'exposure potential' of chemical substances, describing, explaining and predicting how and why different chemicals behave differently in the environment, depending on their physical and chemical substance properties.

Toxic pressure calculation

The concept of toxic pressure calculation was introduced by environmental scientists in Europe to measure the ecological risk of a chemical substance in an (aquatic) system as the probability that exposure concentrations of organisms exceed concentration levels that are considered to be too high or 'riskful' (Posthuma et al., 2002). In this case study, toxic pressure is defined as the probability that expected concentrations of a chemical in 'EU water' are greater than a selected critical effect concentration, HC50-acute (HC=Hazardous Concentration, as derived from a Species Sensitivity Distribution model), for the chemical considered; other definitions of the critical effect concentration can be used for various regulatory purposes, but for the comparisons of mixture toxic pressures to other studies we utilized the HC50-acute. Representing a probability, toxic pressure is expressed as a dimensionless number between zero and one, with higher values implying higher probability to cause harm, related to the selected ecotoxicity endpoint (here: acute-EC50 data). We have adopted the method of toxic pressure calculation as described originally by Van Straalen (2002) and Aldenberg et al. (2002), who calculated exceedance probability from a convolution integral of two distributions, the probability density function of exposure concentrations pdf(C_w), and the cumulative probability function of critical effect concentrations CDF(*HC50*):

$$Toxic\ Pressure = \Pr\{Cw > HC50\} = \int_{-\infty}^{+\infty} pdf(logC_W) \cdot CDF(log\text{HC50})\ dlogC, \qquad (2)$$

known as the 'Van Straalen-Aldenberg integral'. Van Straalen (2002) has used it to calculate the toxic pressure of one single chemical, for which a distribution of exposure concentrations had been observed for a set of field samples, and for which a suite of NOECs test endpoints had been published in the literature. The thus calculated toxic pressure (PAF-NOEC) was interpreted as the fraction of biological species, exposed to above-NOEC concentrations of this chemical. This fraction of species was named later 'Potentially Affected Fraction' (PAF), by Traas et al. (2002), as the parameter quantifying the toxic pressure exerted by an environmental compartment (e.g., water) to a species assemblage; i.e., it is a qualification of the environmental status (to pose harm), not of the species inhabiting that environment. Aldenberg et al. (2002) applied the integral to concentrations of different chemicals, after standardization to averages and standard deviations of the NOECs of the different substances, so effectively applying the concept of concentration addition in calculating exceedance probability. Aldenberg interpreted the outcome as the fraction of species exposed to above-NOEC concentrations of one or more chemicals in the mixture. Traas et al. (2002) and De Zwart and Posthuma (2006) later named Aldenberg's result 'multiple-substance Potentially Affected Fraction' (msPAF).

For this case study, we have borrowed across-species averages of acute EC50s (so-called HC50s) of chemical substances, published by SOLUTIONS-WP18 (in prep.) and calculated standard deviations of these among the different chemical substances studied, in order to obtain standardized distributions exposure- and critical effect concentrations (Table SI-3, Supporting Information). Following Aldenberg's approach, we have applied the Van Straalen-Aldenberg integral of eq 1 to toxicologically standardized distributions of single or multiple chemicals under uncertainty:

$$Toxic\ Pressure = \Pr\{Cw > HC50\} = \int_{-\infty}^{+\infty} pdf(zCw) \cdot CDF(zHC50)dz, \text{ with}$$
$$z(Cw) = \frac{\log(Cw) - average(logHC50)}{standard\ deviation\ (logHC50)}, \text{ and } z(HC50) = \frac{\log(HC50) - average(logHC50)}{standard\ deviation\ (logHC50)}, \qquad (3)$$

as shown in Figure 3. The outcome is to be interpreted as the fraction of all chemicals present, for which exceedance of the HC50-acute is to be expected. This is equivalent to the fraction of occurrences in the hypothetical 'EU water' (places, times) that in which such is the case. As such, this exceedance probability can be used as a measure of expected ecological impact or 'expected risk', as meant by Van Straalen (2002) and Aldenberg et al. (2002), albeit with a slightly different ecological meaning than the 'Potentially Affected Fraction of species' (msPAF), meant by Traas et al. (2002). The outcomes of this assessment are compared to other data on mixture toxic pressure evaluations, of predicted or observed concentrations of chemicals, in order to evaluate the emission modelling approach without dependence on the over-all SOLUTIONS model train (local concentration predictions) results, whilst liaising to and utilizing European regulatory-based models (ECHA, 2016) to predict steady-state concentrations.

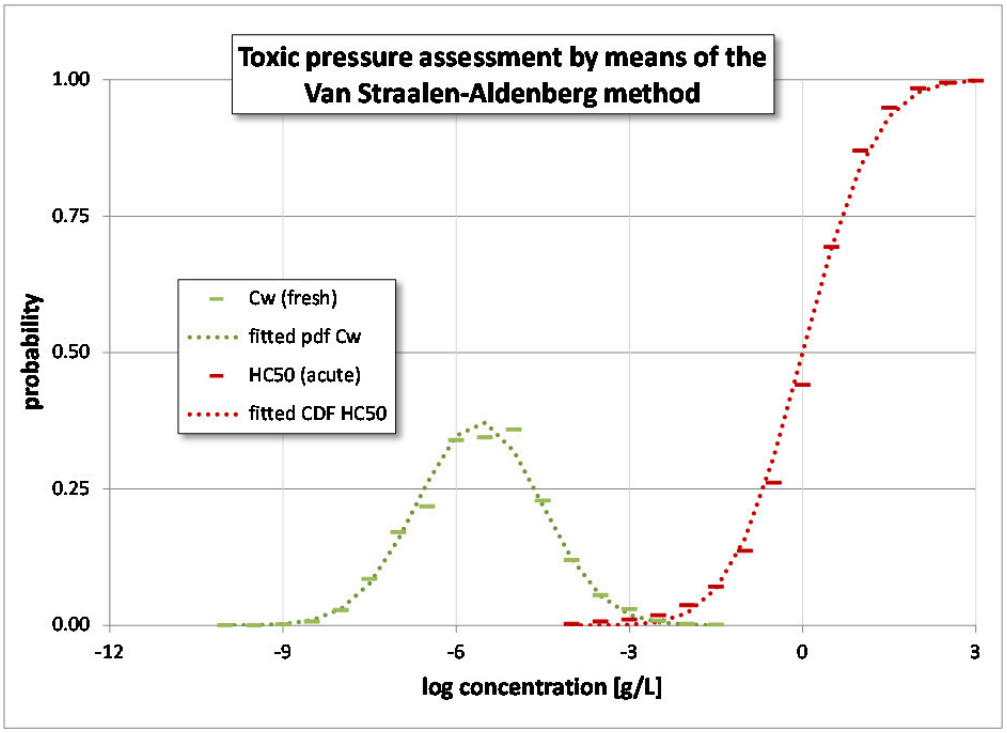

Figure 3. Illustration of the toxic pressure calculation by means of the Van Straalen-Aldenberg integral. Probability of exceedance of critical effect concentrations in 'EU water' Toxic is obtained from the overlap of the probability density function of exposure concentrations pdf(c_W), (green, left) with the cumulative distribution function of critical effect concentrations CDF(HC50), (red, right).

RESULTS and DISCUSSION

Overview

The data collection encompassed more than 12,000 compounds currently in use. The screening-level emission assessment succeeded for 6409 compounds. The numbers of chemicals in various subgroups, the amounts of chemicals used in Europe and their estimated emissions are summarized in Table 2, together with the expected exposure concentrations and expected toxic pressures, which were calculated to test the plausibility and functionality of the emission estimation procedure (according to the *Evaluation 1* and *Evaluation 2* assessments).

Production and Use volumes

Amounts of chemical substances currently used in Europe are shown in the first columns of Table 2. Detailed results, i.e. results for individual chemicals are listed in Table SI-2 (Supporting Information). For reasons of confidentiality, tonnages of individual chemical substances cannot be shared. Histograms of amounts of chemical used in Europe are shown in Figure 4.

Table 2. **Numbers and amounts of chemical substances used in Europe, and their expected concentrations and toxic pressures in 'EU water'.**

	Number of substances	Registered tonnage [tpa]				Estimated emission [tpa]				Expected conc [g/L]			Expected toxic pressure [-]				Pareto ratio
		2.5-p	50-p	97.5-p	sum	2.5-p	50-p	97.5-p	sum	2.5-p	50-p	97.5-p	2.5-p	50-p	97.5-p	total	
REACH mono constituent organics	*3940*	*1.7E-13*	*3.9E-09*	*1.2E+08*	*2.7E+08*	*6.8E-13*	*3.9E-09*	*1.7E-01*	*1.6E+08*	*4.5E-12*	*1.8E-09*	*7.6E-07*	*1.4E-15*	*3.9E-09*	*1.4E-04*	*20%*	*97-3*
REACH more mono constituent organics (not in MLoS)	*182*	*1.7E+00*	*4.9E+02*	*2.9E+04*	*2.9E+06*	*8.0E+00*	*7.4E+02*	*4.1E+04*	*5.8E+05*	*6.4E-11*	*1.9E-08*	*1.2E-06*	*2.1E-12*	*4.0E-07*	*2.5E-04*	*3.2%*	*95-5*
REACH mixed (UVCB) organics (not in MLoS)	*1144*	*6.6E+00*	*9.1E+02*	*2.8E+05*	*5.4E+07*	*1.1E+01*	*8.9E+02*	*2.2E+05*	*3.3E+07*	*2.6E-10*	*3.6E-08*	*1.1E-05*	*5.3E-11*	*1.2E-06*	*3.6E-03*	*44%*	*91-9*
REACH petroleum products (not in MLoS)	*326*	*1.3E+02*	*3.6E+05*	*5.8E+07*	*1.9E+09*	*6.7E+02*	*3.9E+05*	*2.6E+07*	*1.1E+09*	*4.9E-12*	*1.4E-08*	*2.2E-06*	*1.7E-15*	*2.2E-07*	*5.9E-04*	*1.7%*	*89-11*
PHARMA active ingredients of medicines	*397*	*7.6E-05*	*8.2E-01*	*2.7E+02*	*2.5E+04*	*9.3E-07*	*2.8E-02*	*1.7E+01*	*2.5E+04*	*3.7E-17*	*2.4E-12*	*4.6E-09*	*8.2E-34*	*2.3E-16*	*2.7E-08*	*0.01%*	*99-1*
PEST active ingredients of plant protection products	*420*	*6.9E-01*	*5.8E+01*	*2.4E+03*	*1.8E+05*	*6.9E-01*	*5.8E+01*	*2.4E+03*	*1.8E+05*	*4.3E-12*	*9.4E-10*	*1.6E-07*	*1.2E-15*	*9.5E-10*	*1.5E-05*	*0.68%*	*98-2*
ALL ambient mixture in downstream section of river catchmenrt	*6409*				*2.2E+09*				*1.3E+09*	*5.2E-11*	*8.8E-09*	*2.5E-06*	*9.5E-12*	*2.4E-07*	*7.6E-04*	*58%*	*95-5*

Tpa=ton per annuum. Toxic pressure: expressed as msPAF-EC50(acute), derived from SSD-EC50-acute modelling. MLoS=SOLUTIONS 'Modellers List of Substances', a list that compiles data identities and the types of data available per chemical (for a full SOLUTIONS-model train exposure and impact assessment, all parameters required for all modelling steps would be required for all substances, but this is not always the case). UVCB= Chemical Substances of Unknown or Variable Composition, Complex Reaction Products and Biological Materials. PEST=pesticides, PHARMA=pharmaceuticals. Pareto-ratio: see text.

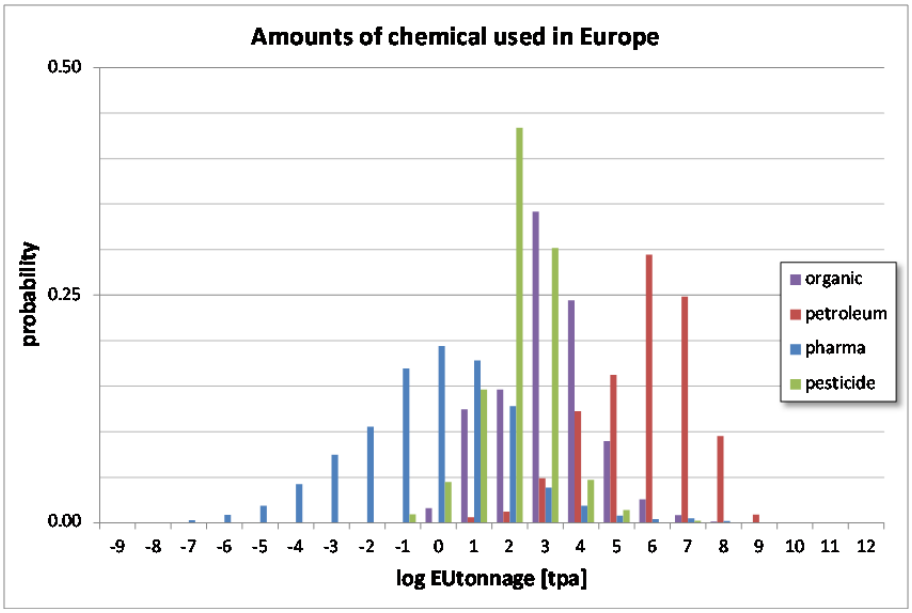

Figure 4. Amounts of chemical substances used in Europe. Use volumes vary from as little as grams per year (pharmaceuticals) to nearly a billion tons per year (petroleum products).

REACH substances. According to the REACH registrations per April 2015 (RIVM, 2015), a total mass of 3.14×10^9 tons of chemical substances are marketed annually in the European Union. EU tonnages were obtained for 12,891 different chemical substances, of which 6,409 substances (representing 2.2×10^9 tons, or 70% of the total mass) could be handled with available REACH-compatible environmental fate models. Of these, 3,940 substances (2.7×10^8 tons or 8 mass%) were relatively simple mono constituent organic substances (in REACH terminology), of which expected concentrations in 'EU water' could be predicted by means of the SimpleBoxTreat model.

Pharmaceuticals. Active ingredients of medicines are produced and used in much lower numbers and masses. Use volumes of 397 different pharmaceuticals, representing 2.5×10^5 tons (0.001 mass%) are listed.

Pesticides. The same holds for active ingredients of crop protection products: 420 chemicals, representing 1.8×10^5 tons (0.006 mass%) are listed.

Overview. The collated data set show that use volumes vary greatly (from as little as 10^{-6} tpa to over 10^9 tpa), both among different groups of chemicals and among individual chemicals within groups. Pharmaceuticals and pesticides are used, both in numbers and amounts, in relatively lower quantities. Consumption volumes range as low as grams per year - pharmaceuticals are typically used in milligrams of active chemical per inhabitant per year. By far the greatest amounts of chemical substance is registered under REACH as petroleum product (1.9×10^9 tons, 60 mass%). Millions of tons per year of petroleum products are produced and used in products such as gasoline and diesel fuel.

Estimated emissions

Emission rates were estimated for all chemical substances listed in Table 2 and Table SI-2 (Supporting Information). Results have been delivered to the Environmental Fate Modeling Team of the SOLUTIONS project, to be used as starting point for assessment of exposure concentrations and ecological impacts of toxic substances in EU river catchments[4].

The results of the emission estimation modelling are presented below, and have been evaluated in this study to test the plausibility and functionality of the generic emission estimations by means of the two evaluation efforts. Although petroleum products and other less well defined chemical substances are not considered in the SOLUTION project, these substances are included in the exploratory case study of the *Evaluation-2* assessment, because their possible impacts on ecosystems cannot be ignored without further consideration.

Overview of emission model outcomes. Emissions have narrower ranges than use volumes. As shown in Figure 5, estimated emission rates span a range of roughly 10 orders of magnitude: 10^{-5} tpa to 10^{5} tpa. The main reason is the high-volume uses happen to have relatively low release fractions. As reported by the European Oil Refinery branch organization Concawe to the European Chemicals Agency ECHA in REACH Chemical Safety Assessments (Concawe, 2008), fractions of fuel, released unburnt from vehicles, are generally below 0.1%. In contrast, the lower-volume used chemicals (pharmaceuticals and pesticides) have relatively high release fractions. Pesticides are nearly entirely released to the environment in open-field uses.

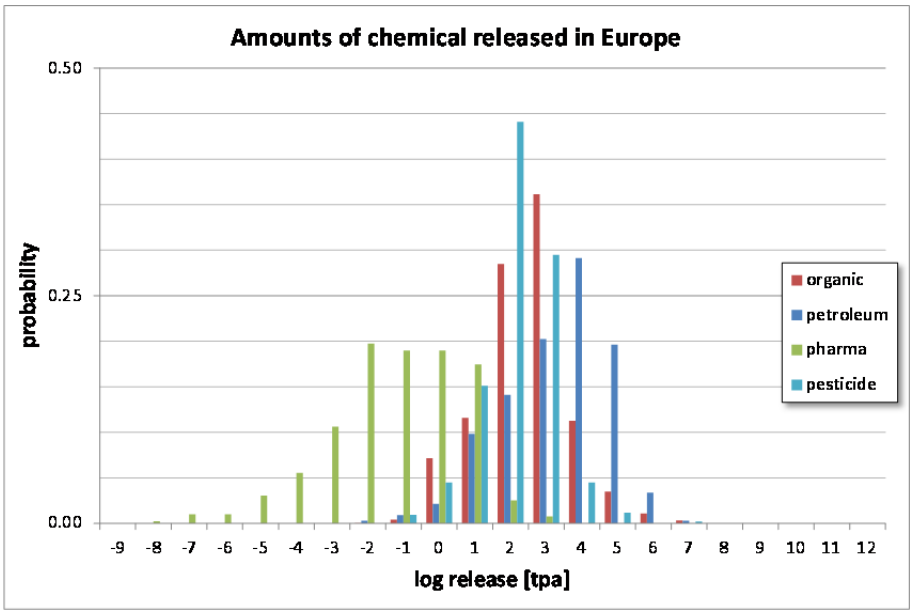

Figure 5. Estimated amounts of chemicals released to the environment in Europe.

[4] Reported in D14.2 (in prep.)

Results evaluation 1, exposure: predicted and observed concentrations

Van Gils et al. (in prep.) extensively compared predicted and observed environmental concentrations in selected European surface waters. This evaluation is made possible by combining the generic emission model outcomes with detailed fate modelling, and thereupon comparing predicted and observed concentrations. Their preliminary conclusion can be characterized as follows:

- There seems to be no systematic bias between the outcome SOLUTIONS model train (which combines emission estimates and fate modelling) and measured concentrations that are over all studied compounds less than one order of magnitude for 65% of the chemicals that could be studied (for which surface water concentrations were available) and less than two orders in 90% of cases
- Over- and under-predicted concentrations were evenly distributed

This result is not surprising. It is entirely in line with Forbes' (2010) observation that 'Although we may be right on average, we may be wrong most of the time'. This result seems to confirm the claim that the SPERC tables proposed by industry (Cefic, 2012) represent reasonably accurate estimates of fractions released in various uses, so that in this situation, the SOLUTIONS model train is 'right on average' (i.e. right on average, given the enormous differences among different chemicals) . This result is pleasantly surprising in the sense that the outcomes of the SOLUTIONS model train, while certainly being 'wrong most of the time', are often reasonably close to the measured values. However, the same results function in a context with uncertainties of similar magnitude, such as (1) the commonality of use of an application factors ranging 1, 2 and 3 orders of magnitude for e.g. derivation of an Environmental Quality Standard from available data, or (2) the wide spatial and temporal variability of measured concentrations used as 'anchor' for this validation step. The most promising observation is that the median of the bias in the predicted-observed comparison of concentrations is very close to neutral (i.e. no bias observed!, see Van Gils et al., D14.2, in prep.)[5]. Note that the results of the evaluation of predicted and observed concentrations were obtained after removal of the volatile compounds from the data set, related to specific discrepancies.

Results Evaluation 2 - impacts: Expected concentrations and mixture toxic pressure

Expected concentrations

Expected concentrations in 'EU water', calculated from estimated emission rates with SimpleBoxTreat, are also shown in Table 2 and Table SI-2 (Supporting Information). Predicted concentrations in the 'EU water' span an even narrower range than emissions. When the extremely low expected concentrations of pharmaceuticals are excluded the range is limited to roughly 6 orders of magnitude: from picograms per liter to micrograms per liter (Figure 6). This is in agreement with earlier observations of Zijp et al. (2014), who predicted similar concentration distributions in Rhine water, and found these to match available observations. They reported that, with some notable exceptions – some high observations were not predicted, perhaps because of unexpectedly high emissions, whereas very low concentrations did not seem to occur or have remained undetected – concentrations of organic chemicals dissolved in Rhine water, are mostly in the lower microgram per liter range, which was also predicted from

[5] This section will be expanded upon finalisation of D14.2, which provides important insights in the net accuracy of emission + fate model outcomes.

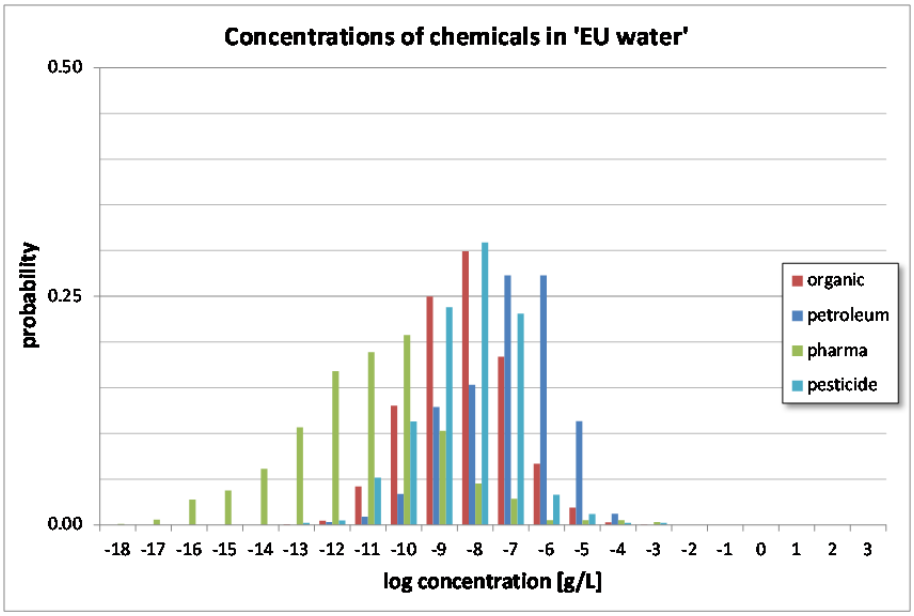

Figure 6. Expected concentrations of chemical substances in regional fresh waters in Europe, derived as defined in ECHA (2016).

estimated emissions by means of multi-media environmental fate modeling. Despite estimations in the correct (wide) range, Zijp's per-chemical predictions did not seem to correlate well with observations, confirming again the correctness of Forbes' statement (Forbes, 2010) about being 'right on average, but wrong most of the time'. The observed uncertainties are small enough not to exclude useful application of the calculated distributions of exposure concentrations in toxic pressure calculation by means of the Van Straalen-Aldenberg integral under uncertainty.

Expected toxic impacts

Toxic pressures, calculated from estimated emissions and modeled exposure concentrations with eq 3, are summarized in Table 2. Expected toxic pressures of net 6,409 substances considered in this case study are listed in Table SI-3 (Supporting Information).

Direct ecological impacts of many individual chemicals on aquatic ecosystems, here considered as the 'EU water' in steady-state conditions regarding eventual chemical concentrations as expected from estimated emissions, are characterized by low toxic pressure values (PAF-EC50 acute). Probabilities of exceeding critical effect concentrations (EC50-acute), as apparent from median values for the various categories of chemicals, are all below the 10^{-6} range: it is less than 0.0001% probable that HC50 (i.e. across-species average EC50) is exceeded in one or more situations (times, places) in the water body considered, which is the same as saying that this is the case for less than 0.0001% of the species present, which is the same as saying that it is 0.0001% probable to find a species for which EC50 is exceeded anywhere, anytime in 'EU water'. *With emphasis,* note that this assessment outcome is *not* reflecting the consequences of emissions close to their source; for those situations either measured concentrations or the SOLUTIONS-model train can provide spatio-temporal refined outputs (see D14.2). It can also be seen from Table 2, however, that the predicted toxic pressures of a considerable (i.e. non-negligible) fraction of the 6000^{+} chemical substances considered in this case study is estimated as values that cannot be interpreted as relatively low in the aforementioned interpretation. Notably, 97.5

percentiles (right margins of 95% confidence intervals) of some categories of the REACH substances exceed values known from other studies to imply impacts on species assemblages. This is the case, for example, for the REACH category of 'mixed (UVCB) organics', in which 28 of the 1144 substances have expected toxic pressures (PAF-EC50) greater than 0.04%, and for which the combined toxic pressure metric (msPAF-EC50-acute) amounts to 40% according to the present modelling sequence (emission model + generic fate model + hazard model + mixture model). Use of REACH-registered UVCB organics – these 'difficult' chemicals are not considered in the SOLUTIONS project, but included in this case study – is expected to lead to a concern-raising probability that critical effect concentrations may be exceeded in 'EU water'. To a somewhat lesser extent, this also holds for the REACH category of 'mono constituent organics' (i.e. 'ordinary', 'well-modeled' substances cf. the evaluations of predicted and observed concentrations of Van Gils et al, D14.2), of which exceedance of critical effect concentrations is 20% probable for the 'EU water' under predicted steady-state conditions.

As can be seen from Table 2 as well, relatively limited direct impacts on species assemblages are to be expected from substances in the REACH category of petroleum products. Although this category contains substances with high production and use tonnages, little of this is released in its original form to the environment, while dissolved concentrations in water tend to remain low as a result of extremely low water solubility whilst toxicity is relatively low. Expected toxic pressures of petroleum products are expected to be relatively small (msPAF-EC50 of petroleum products in steady state ≈ 1.7%), in spite of the large amounts of these chemicals produced and used.

Relatively low values of toxic pressure estimates (PAF-EC50) in steady state 'EU water' were also found for the non-REACH categories of chemical substances (pharmaceuticals and pesticides). Non-negligible toxic pressures are expected for a small number of pesticides only, leading to an expected combined toxic pressure of 0.7%. Above-negligible toxic pressures in steady state 'EU water' are not expected for any of the pharmaceuticals considered in this study. Again, it should be noted that these outcomes are of a generic kind, and applicable for a European-scale assessment. End-of-pipe concentration patterns, and spatio-temporally explicit assessments, show different patterns of relative importance of chemicals.

The results of this case study are in fair agreement with various earlier studies, in which specific attention can be paid to two phenomena: (1) the distribution range of mixture toxic pressures for an array of sampling sites or water bodies, and (2) the relative contribution of individual chemicals, or chemical groups, within the total mixture to the mixture toxic pressure. Regarding these aspects, the current outcomes for the 'EU water in steady state' are in fair agreement with the recent findings of De Zwart and Posthuma (2016), who estimated mixture toxic pressures from chemical monitoring data in fresh waters in the Netherlands. They found that, generally, (i) toxic pressures in fresh waters are in the same range as found in the present study, and that (ii) toxic pressures, based on measured exposure concentrations, can generally be attributed to a relatively low number of chemicals. This corroborates a suite of other studies, in which it was commonly found that a mixtures' impact can commonly be attributed to a relatively low number of chemicals, found in various types of studies and various geographies, and for various compound groups (e.g., Backhaus and Karlsson, 2014 for pharmaceuticals in European coastal waters; Vallotton and Price, 2016, for pesticides in the US, and Posthuma et al., 2016 for a suite for chemicals in Dutch surface waters). Most significantly, this case study reconfirms

one of the earliest findings of this kind (Harbers et al., 2006) that generally, only small fractions of the chemicals produced, used and emitted are responsible for the larger part of the direct ecological impacts for a particular situation. Note, within this pattern, that the dominant chemicals vary with scale (e.g., from an 'EU water' in steady state to a local water body with a typical emission source nearby) and time (e.g., pesticides in- and outside the cropping season). This outcome pattern can be summarized as a Pareto effect, also known under its most frequently-cited outcome "the 80-20 rule'". Although this should be immediately evident from the probability calculation which underlies the toxic pressure derivation by the Van Straalen-Aldenberg integral, the notion that toxic pressures stem from overlaps of tails of distributions and should (therefore) be expected to be Pareto distributed seems not to be shared widely, in spite of the many studies reporting such findings and many phenomena in the physical world reflecting this phenomenon (Newman, 2007; West, 2017). Pareto-findings are commonly (but incorrectly) referred to as always obeying to the '80-20 rule', while in reality often deviating Pareto ratios are reported. In this case study, we found Pareto ratios (much) greater than 90-10 (table 2). For the 'ordinary' (mono constituent) REACH chemicals, a '95-5 rule' was found. Note that the continuous, heavily tailed Pareto distribution (here: with many relatively low values, and few high values) can be interpreted as a continuum (ranking here the relative potential of chemicals to pose harm in a EU water body in steady state), or as outcomes that allow classification (e.g. a class of chemicals unlikely to pose harm in the EU water body, and a class that might pose harm). Such assessments have also been made, based on different degrees of model focus (e.g., emissions, hazard) and approaches, and for other endpoints (e.g., Ahrens et al., 2016, Oltmanns et al., 2018, Schulze et al., 2018).

Uncertainty and mixture toxicity, and relevance for emission estimation modelling

This impact evaluation case study has revealed that use of the Van Straalen-Aldenberg method of toxic pressure calculation has two useful consequences: (i) the ability to quantitatively account for uncertainty in assumed input data and (ii) the ability to quantify (combined) toxic pressures of mixtures. The latter has been pointed out by Aldenberg et al. (2002) already, by showing how this can be done for substances with equal standard deviations of EC50's across species. We have demonstrated that it is mathematically correct to apply the Van Straalen-Aldenberg integral for calculating exceedance probability to all chemicals, regardless their inter-species variance of EC50 (Van de Meent et al., 2018). Whilst focusing on the *Evaluation-2* outcomes to validate the emission model, this case study has also shown the functionality of it in assessment of toxic pressures of complex mixtures of chemicals. The first and perhaps most important consequence of this seems to have remained undiscovered. Although both Van Straalen (2002) and Aldenberg et al. (2002) have been aware of the essence of the method, *viz*. exceedance probability being described as the mathematical quantification of overlap of two distributions, neither of them have pointed out the significance of this for treatment of uncertainty. This important aspect of toxic pressure calculation from the overlap of distributions became clear to us while trying to assess the possible influence of uncertainty in estimated emissions and modeled exposure concentrations on the expected impacts of ambient mixtures of chemicals in larger water bodies. It is clear from equation 3 and Figure 3 that wider distributions of exposure concentrations (other things remaining equal) have greater overlap with the (standard-normal) distribution of critical effect concentrations than narrow distributions. This is particularly clear when considering the exceedance probability of one single concentration of one single chemical with and without uncertainty.

It is clear that adding uncertainty to the one exposure concentration widens the distribution of possible true values of the exposure concentration, thereby increasing the probability of having concentrations that exceed possible values of the critical effect concentrations. Although perhaps less obvious, the same is true for mixtures: adding uncertainty about the true values of the modeled concentrations of the various chemical components of the mixture adds probability of exceeding critical effect concentrations. By quantifying exceedance probability from overlap of distributions, uncertainty has thus implicitly been accounted for via the influence of uncertainty on the width of the distribution of exposure concentrations. Interpretation of the outcome of the Van Straalen-Aldenberg convolution integral should thus be that this is the conditional probability, given the uncertainties in the elements that make up the distributions to which the convolution is applied, of having exposure concentrations that exceed critical effect concentrations.

These findings bear important lessons on the implicit idea that all modelling steps should seek high precision for all purposes of foreseen use in water quality protection, assessment and management. Although precision is certainly desired from a scientific perspective, there current study illustrates that a realistic approach, based on available (often lacking) data can provide useful screening insights for management. That is, we have studied – Van de Meent et al. (2017); results not shown here – the influence of uncertainty in quantifying mixture toxic pressures of REACH substances by means of Monte Carlo simulation, and (focusing on emission uncertainties) discovered that the quantitative influences of emission uncertainties are much smaller than anticipated. The explanation (in hindsight) is that distributions of exposure concentrations of ambient mixtures are very wide already (many orders of magnitude, Figure 5) so that adding uncertainty to input elements (emission estimates!) adds little to the overlap which exists already. Another way of looking at this is to realize that emission estimation is so uncertain that distributions of exposure concentrations, modeled from these emissions, contain this uncertainty already. One could say that toxic pressure calculations of modeled concentrations under uncertainty implicitly account for this uncertainty, when looking at the scale and time characteristics studied here. The significance of this for impact assessment of mixtures of toxic substances under uncertainty is that mixture toxic pressures can be relatively well known without assessing the toxic pressures of the components of the mixture first. That is, a first-tier toxic pressure calculation can be done directly from knowledge of the parameters of the distributions of exposure concentrations and critical effect concentrations, to establish (mixture) toxic pressures for a scale like considered here, the 'EU water' (defined in ECHA, 2016). Values of these parameters (averages, standard deviations) can often be inferred having detailed and highly precise knowledge of exposure concentrations. For the required accuracy and precision of emission estimation, this means that, paraphrasing Forbes' statement, 'we can afford to be wrong most of the time, as long as we are right on average' in the first-tier assessment of net risks of chemicals. As stated above, the SOLUTIONS-modelling approach refines on this, by considering a higher-tier approach with spatio-temporally explicit modelling of exposures and risks. The present results imply, that a two-tiered approach – first focusing on a chemo-centric screening-level approach to the evaluation of the potential of very many chemicals to pose harm according to the approach presented in the present paper and aligned with ECHA (2016) and then applying a refined assessment for the compounds that are identified to potentially cause harm according to the SOLUTIONS approach – may be a pragmatic and informative approach to handling the problem of >100,000 chemicals.

Conclusions

We conclude that the emission rates of chemicals used in Europe can be estimated with sufficient accuracy and precision to allow assessment of expected impacts of the use of these chemicals on aquatic ecosystems in a way useful for a screening-level estimation of release rates in the context of chemical and environmental risk assessment and management. This overall conclusion is based on developing and describing an emission estimation approach that would enable estimating emission rates for a vast number of chemicals with a realistic set of (relatively minimal) data. The accuracy of the emission model was evaluated, and compared with two (derived) evaluation variables, being measured ambient concentrations and mixture toxic pressure results from other studies. The predicted-observed comparison at the level of ambient concentrations resulted in the observation that the net results of emission+fate modelling are in fair agreement with observed chemical concentrations. The predicted mixture toxic pressure of an 'EU water body' in steady state was in fair comparison to other studies on mixture toxic pressures and other mixture analyses, especially reflecting that the predicted mixture toxic pressure reflect an exposure level range that implies that surface waters are likely subject to a chemical mixture pressure, and that the underlying per-chemical toxic pressure data are Pareto-distributed. That is, the relative contributions of chemicals to ecological impacts appeared to be distributed in a heavily-tailed (Pareto-) distribution, with a larger fraction chemicals exhibiting relatively low and a smaller fraction of chemicals exhibiting relatively high predicted impacts. The latter is a direct consequence of the wide across-chemicals distributions of production and emission masses and associated predicted concentration variability collated in the present paper. The results can be summarized as a screening-level approach, via which chemicals can be assigned to a group with (very) low probability to cause harm in an 'EU water' in steady state, and a group with a relatively higher probability to do so. The latter group can be subject to a refined assessment, as developed in the SOLUTIONS-project in the format of a full spatio-temporally explicit assessment of chemical risks and impacts. We argue that the screening-level assessment can be used to effectively run the refined assessment, given the vast number of potentially relevant compounds being >100,000; a similar approach and use of outcomes has been promoted (with slightly different inputs and approaches) by various other scholars. We finally emphasize that the approach presented in the present study is in line with the holistic nature of the Water Framework Directive, which has been built on watersystem-level principles. That is, the current study provides a screening-level and systems-oriented approach to sub-select chemicals for management on the European scale, which can be followed by a site- and substance oriented approach in chemical management if needed. This approach vastly expands on the opportunities of the approaches focusing on single chemicals, addressed separately.

Acknowledgements

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TABLES AND FIGURES

Table 1. Estimated release fractions in the various uses and life cycle stages. Based on published and unpublished reports. (spERC = Specific Environmental Release Category)

Activity category		release	to air	to water	to soil
Stage I	Use1: MANUFACTURING [1]	0.4%	0.2%	95%	5%
Stage I	Use2: DISTRIBUTION & FORMULATION [1]	0.5%	60%	39%	1%
Stage I	Use3: INDUSTRIAL PROCESSING [1]	0.5%	59%	35%	6%
Stage II	Use4: USE in AGRICULTURE [2]	100%	15%	1%	84%
Stage II	Use5: USE in MEDICINE [3]	12%	0.0%	100%	0%
Stage II	Use6: WIDE-DISPERSIVE USE in 'down-the-drain' [1]	100%	0.0%	100%	0%
Stage II	Use7: Other WIDE-DISPERSIVE USES [1]	100%	73%	11%	16%
Stage II	Use8: WIDE-DISPERSIVE 'low-release' USES [1]	5%	73%	11%	16%
Stage II	Use9: USE as FUEL [4]	0.04%	96%	4%	0%
Stage II	Use10: Other stage-II USES [1]	0.5%	26%	22%	9%
Stage III	Use11: TREATMENT, RECYCLING [1]	5%	33%	33%	33%
Stage III	Use12: SOLID WASTE DISPOSAL [1]	10%	0.0%	0.0%	100%
Use-weighted averages, based on selected spERCs		25%	63%	31%	6%

[1] Cefic, 2012

[2] Sala et al., 2014, 2015

[3] IKBR, 2009; Fent et al., 2006; Van der Aa et al., 2008,2011

[4] Concawe, 2008

Table 2. Numbers and amounts of chemical substances used in Europe, and their expected concentrations and toxic pressures in 'EU water'.

	Number of	Registered tonnage [tpa]				Estimated emission [tpa]				Expected concentration [g/L]			Expected toxic pressure [-]				Pareto
	substances	2.5-p	50-p	97.5-p	sum	2.5-p	50-p	97.5-p	sum	2.5-p	50-p	97.5-p	2.5-p	50-p	97.5-p	total	ratio
REACH mono constituent organics	*3940*	*1.7E-13*	*3.9E-09*	*1.2E+08*	*2.7E+08*	*6.8E-13*	*3.9E-09*	*1.7E-01*	*1.6E+08*	*4.5E-12*	*1.8E-09*	*7.6E-07*	*1.4E-15*	*3.9E-09*	*1.4E-04*	*20%*	*97-3*
REACH more mono constituent organics (not in MLoS)	*182*	*1.7E+00*	*4.9E+02*	*2.9E+04*	*2.9E+06*	*8.0E+00*	*7.4E+02*	*4.1E+04*	*5.8E+05*	*6.4E-11*	*1.9E-08*	*1.2E-06*	*2.1E-12*	*4.0E-07*	*2.5E-04*	*3.2%*	*95-5*
REACH mixed (UVCB) organics (not in MLoS)	*1144*	*6.6E+00*	*9.1E+02*	*2.8E+05*	*5.4E+07*	*1.1E+01*	*8.9E+02*	*2.2E+05*	*3.3E+07*	*2.6E-10*	*3.6E-08*	*1.1E-05*	*5.3E-11*	*1.2E-06*	*3.6E-03*	*44%*	*91-9*
REACH petroleum products (not in MLoS)	*326*	*1.3E+02*	*3.6E+05*	*5.8E+07*	*1.9E+09*	*6.7E+02*	*3.9E+05*	*2.6E+07*	*1.1E+09*	*4.9E-12*	*1.4E-08*	*2.2E-06*	*1.7E-15*	*2.2E-07*	*5.9E-04*	*1.7%*	*89-11*
PHARMA active ingredients of medicines	*397*	*7.6E-05*	*8.2E-01*	*2.7E+02*	*2.5E+04*	*9.3E-07*	*2.8E-02*	*1.7E+01*	*2.5E+04*	*3.7E-17*	*2.4E-12*	*4.6E-09*	*8.2E-34*	*2.3E-16*	*2.7E-08*	*0.01%*	*99-1*
PEST active ingredients of plant protection products	*420*	*6.9E-01*	*5.8E+01*	*2.4E+03*	*1.8E+05*	*6.9E-01*	*5.8E+01*	*2.4E+03*	*1.8E+05*	*4.3E-12*	*9.4E-10*	*1.6E-07*	*1.2E-15*	*9.5E-10*	*1.5E-05*	*0.68%*	*98-2*
ALL ambient mixture in downstream section of river catchmenrt	*6409*				*2.2E+09*				*1.3E+09*	*5.2E-11*	*8.8E-09*	*2.5E-06*	*9.5E-12*	*2.4E-07*	*7.6E-04*	*58%*	*95-5*

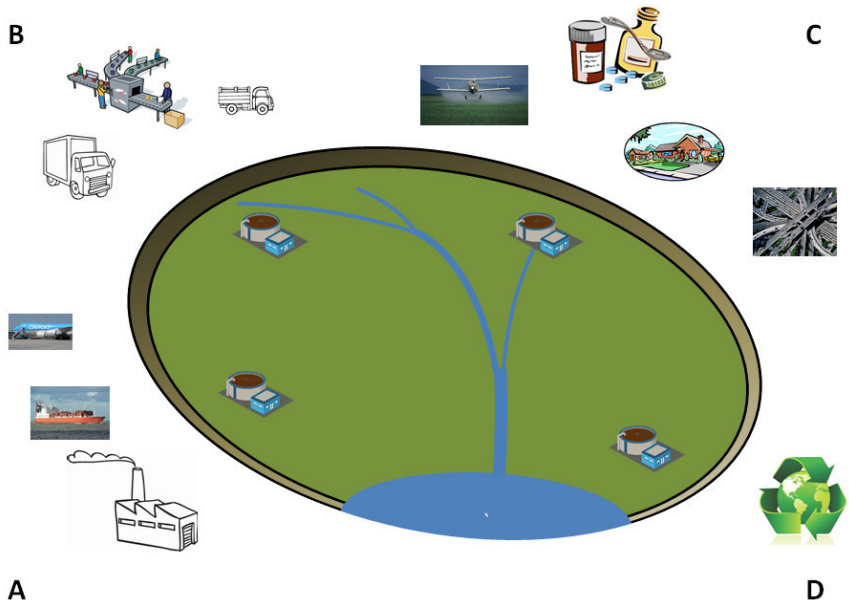

Figure 1. Releases of chemical substances are estimated for a variety of uses in all life cycle stages: manufacturing and transport (A), formulation and distribution (B), service life (C) and recycling/waste stage (D). In most uses, release to the environment takes place after waste water treatment.

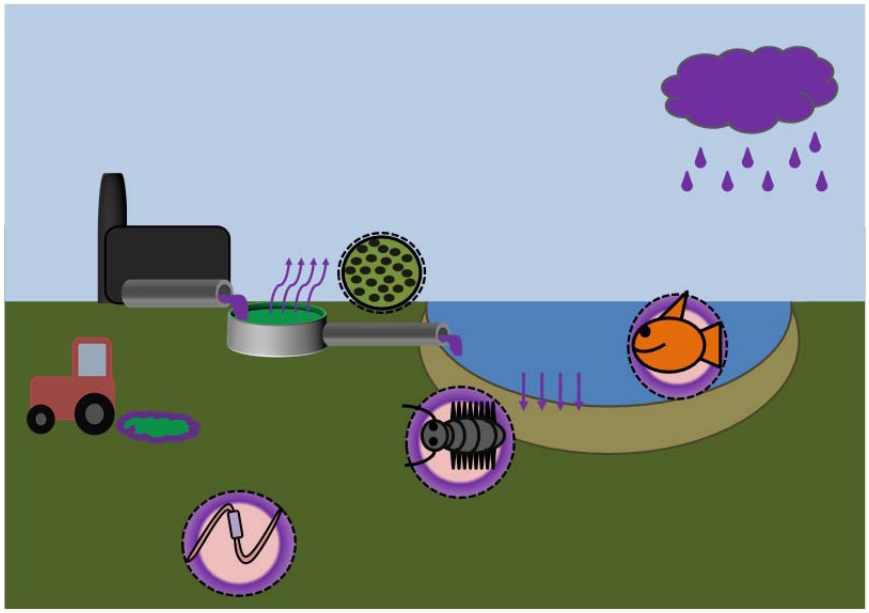

Figure 2. A simplified three-compartment version of the multimedia mass balance model SimpleBox (Hollander et al., 2016), combined with the sewage treatment plant simulation model SimpleTreat (Struijs et al., 2016), is used by the German Federal Environment Office (UBA) to calculate 'exposure potential' of chemical substances, describing, explaining and predicting how and why different chemicals behave differently in the environment, depending on their physical and chemical substance properties.

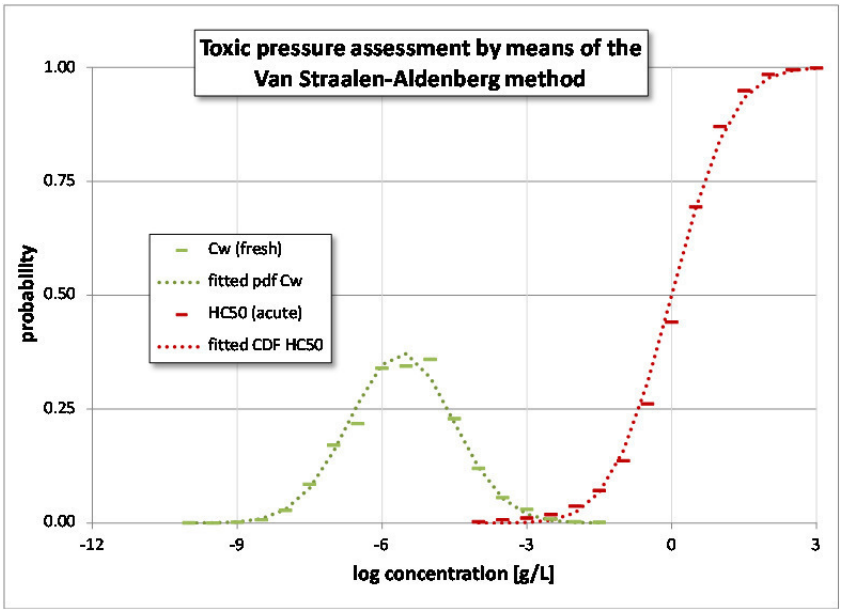

Figure 3. Illustration of the toxic pressure calculation by means of the Van Straalen-Aldenberg integral. Probability of exceedance of critical effect concentrations in 'EU water' Toxic is obtained from the overlap the probability density function of exposure concentrations pdf(c_W), (green, left) with the cumulative distribution function of critical effect concentrations CDF(HC50), (red, right).

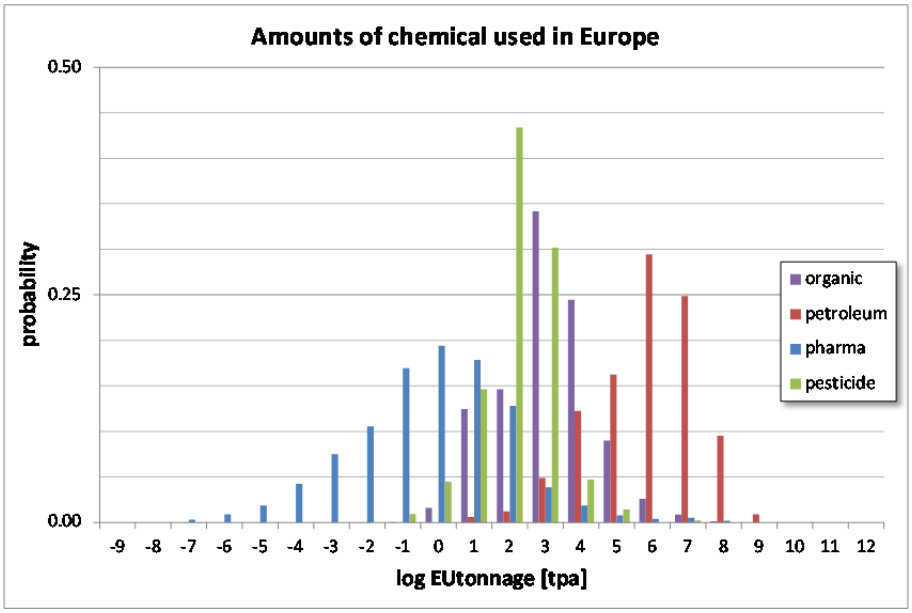

Figure 4. Amounts of chemical substances used in Europe. Use volumes vary from as little as grams per year (pharmaceuticals) to nearly a billion tons per year (petroleum products).

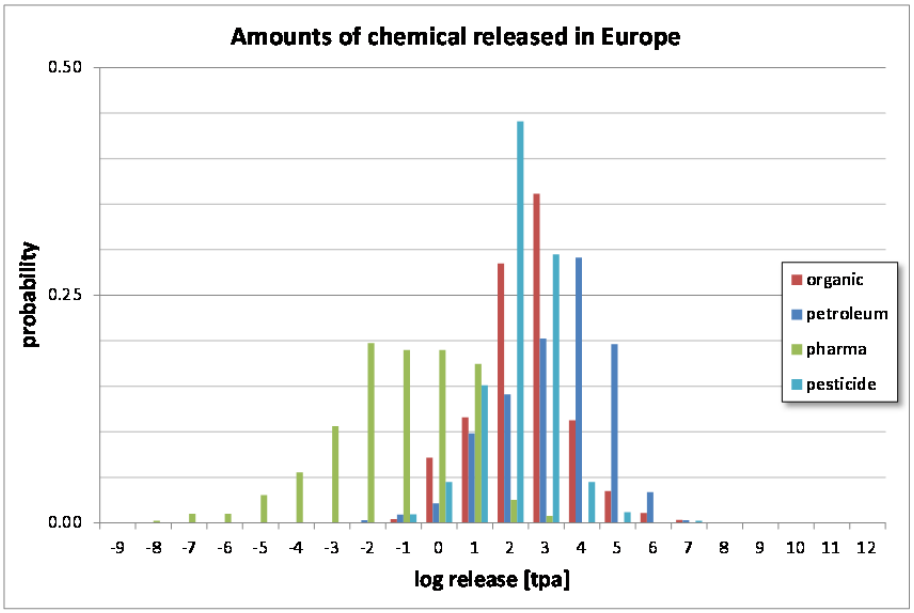

Figure 5. Estimated amounts of chemicals released to the environment in Europe.

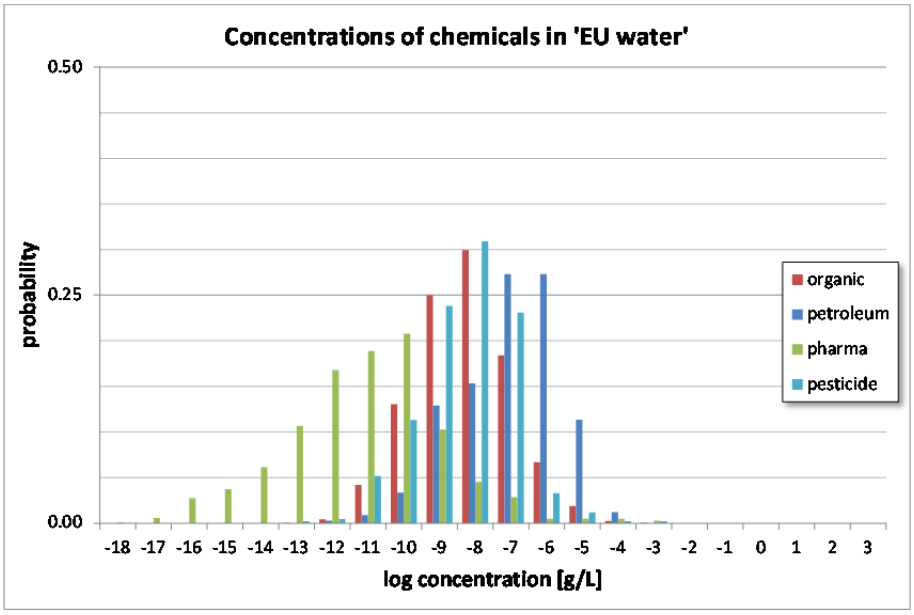

Figure 6. Expected concentrations of chemical substances in regional fresh waters in Europe, derived as defined in ECHA (2016).

SUPPORTING INFORMATION

Table SI-1. Fractions of EU tonnages released in specific Environmental Release Categories, spERC (Cefic, 2012).

SPERC #	SPERC Name	Glossary text	Release fraction to air	Release fraction to waste water	Release fraction to soil	Sum of release fractions
1	AISE SPERC 2.1.a.v1	AISE SPERC 2.1.a.v1 - AISE 1 - Formulation of Detergents/Maintenance Products: Granular Detergent -Regular (large scale)	2.0E-04	1.0E-04	0.0E+00	3.0E-04
2	AISE SPERC 2.1.b.v1	AISE SPERC 2.1.b.v1 - AISE 2 - Formulation of Detergents/Maintenance Products: Granular Detergent -Regular (medium scale)	2.0E-04	1.0E-03	0.0E+00	1.2E-03
3	AISE SPERC 2.1.c.v1	AISE SPERC 2.1.c.v1 - AISE 3 - Formulation of Detergents/Maintenance Products: Granular Detergent -Regular (small scale)	1.0E-02	2.0E-03	0.0E+00	1.2E-02
4	AISE SPERC 2.1.g.v1	AISE SPERC 2.1.g.v1 - AISE 7- Formulation of liqud Detergents/Maintenance Products: Low Viscosity (large scale)	0.0E+00	1.0E-04	0.0E+00	1.0E-04
5	AISE SPERC 2.1.h.v1	AISE SPERC 2.1.h.v1 - AISE 8 - Formulation of liqud Detergents / Maintenance Products: Low Viscosity (medium scale)	0.0E+00	1.0E-03	0.0E+00	1.0E-03
6	AISE SPERC 2.1.i.v1	AISE SPERC 2.1.i.v1 - AISE 9 - Formulation of liqud Detergents/Maintenance Products: Low Viscosity (small scale)	0.0E+00	2.0E-03	0.0E+00	2.0E-03
7	AISE SPERC 2.1.j.v1	AISE SPERC 2.1.j.v1 - AISE 10 - Formulation of liqud Detergents/Maintenance Products: High Viscosity (large scale)	0.0E+00	1.0E-03	0.0E+00	1.0E-03
8	AISE SPERC 2.1.k.v1	AISE SPERC 2.1.k.v1 - AISE 11 - Formulation of liqud Detergents/Maintenance Products: High Low Viscosity (medium scale)	0.0E+00	2.0E-03	0.0E+00	2.0E-03
9	AISE SPERC 2.1.l.v1	AISE SPERC 2.1.l.v1 - AISE 12 - Formulation of liqud Detergents/Maintenance Products: High Viscosity (small scale)	0.0E+00	4.0E-03	0.0E+00	4.0E-03
10	AISE SPERC 4.1.v1	AISE SPERC 4.1.v1 - AISE 13 - Industrial Use of Water Borne Processing Aids - no RMM	0.0E+00	1.0E+00	0.0E+00	1.0E+00
11	AISE SPERC 5.1a.v1	AISE SPERC 5.1a.v1 - AISE 14 - Industrial Use of Me-salts in conversion coating - Nickel	0.0E+00	5.0E-02	0.0E+00	5.0E-02
12	AISE SPERC 5.1b.v1	AISE SPERC 5.1b.v1 - AISE 15 - Industrial Use of Me-salts in conversion coating - Zinc, Chromium, Copper, Manganese	0.0E+00	1.0E-02	0.0E+00	1.0E-02
13	AISE SPERC 8a.1.a.v1	AISE SPERC 8a.1.a.v1 - AISE 16 - Wide Dispersive Use in 'Down the Drain' cleaning and maintenance products (Consumers and Professionals)	0.0E+00	1.0E+00	0.0E+00	1.0E+00
14	AISE SPERC 8a.1.b.v1	AISE SPERC 8a.1.a.v1 - AISE 17 - Wide Dispersive Use in Aerosol products for cleaning and maintenance products (Non-Propellants)	0.0E+00	1.0E+00	0.0E+00	1.0E+00
15	AISE SPERC 8a.1.c.v1	AISE SPERC 8a.1.a.v1 - AISE 18 - Wide Dispersive Use in Aerosol products for cleaning and maintenance products (Propellants)	1.0E+00	0.0E+00	0.0E+00	1.0E+00
16	CEPE SPERC 2.1a.v1	CEPE SPERC 2.1a.v1 - CEPE 1 - Formulation of Organic Solvent Borne Coatings and Inks - Large Scale (>100 tpa solvent use) - VOC	6.0E-03	0.0E+00	0.0E+00	6.0E-03
17	CEPE SPERC 2.1b1.v1	CEPE SPERC 2.1b1.v1 - CEPE 2 - Formulation of Organic Solvent Borne Coatings and Inks - Small Scale (<100 tpa solvent use) - VOC	6.0E-03	0.0E+00	0.0E+00	6.0E-03
18	CEPE SPERC 2.2a.v1	CEPE SPERC 2.2a.v1 - CEPE 3 - Formulation of Organic Solvent Borne Coatings and Inks - Solids	9.7E-05	5.0E-05	0.0E+00	1.5E-04
19	CEPE SPERC 2.1b2.v1	CEPE SPERC 2.1b2.v1 - CEPE 4 - Formulation of Water Borne Coatings and Inks - Large Scale (>100 tpa solvent use) - VOC	4.0E-03	0.0E+00	0.0E+00	4.0E-03
20	CEPE SPERC 2.1b3.v1	CEPE SPERC 2.1b3.v1 - CEPE 5 - Formulation of Water Borne Coatings and Inks - Small Scale (<100 tpa solvent use) - VOC	4.0E-03	0.0E+00	0.0E+00	4.0E-03
21	CEPE SPERC 2.1b4.v1	CEPE SPERC 2.1b4.v1 - CEPE 6 - Formulation of Water Borne Coatings and Inks - Solids	9.7E-05	5.0E-03	0.0E+00	5.1E-03
22	CEPE SPERC 2.1c.v1	CEPE SPERC 2.1c.v1 - CEPE 7 - Formulation of Powder Coatings and Inks - Solids	9.7E-05	5.0E-03	0.0E+00	5.1E-03
23	CEPE SPERC 2.2a1.v1	CEPE SPERC 2.2a1.v1 - CEPE 8 - Formulation of Liquid Coatings and Inks (where specific use not known) - Large Scale (>100 tpa solvent use) - VOC	6.0E-03	0.0E+00	0.0E+00	6.0E-03
24	CEPE SPERC 2.2a2.v1	CEPE SPERC 2.2a2.v1 - CEPE 9 - Formulation of Liquid Coatings and Inks (where specific use not known) - Small Scale (<100 tpa solvent use) - VOC	6.0E-03	0.0E+00	0.0E+00	6.0E-03
25	CEPE SPERC 2.2a3.v1	CEPE SPERC 2.2a3.v1 - CEPE 10 - Formulation of Liquid Coatings and Inks (where specific use not known) - Solids	9.7E-05	5.0E-03	0.0E+00	5.1E-03
26	CEPE SPERC 8c.2.v1	CEPE SPERC 8c.2.v1 - CEPE 11 - Wide Dispersive Application of Decorative Coatings - Consumer and Professionals - indoor use - Solvents and volatiles	9.9E-01	1.0E-02	0.0E+00	1.0E+00
27	CEPE SPERC 8c.1.v1	CEPE SPERC 8c.1.v1 - CEPE 12 - Wide Dispersive Application of Decorative Coatings - Consumer and Professionals - indoor use - Solids	0.0E+00	1.0E-02	0.0E+00	1.0E-02
28	CEPE SPERC 8f.2.v1	CEPE SPERC 8f.2.v1 - CEPE 13 - Wide Dispersive Application of Decorative Coatings - Consumer and Professionals - outdoor use - Solvents and Volatiles	9.9E-01	1.0E-02	5.0E-03	1.0E+00
29	CEPE SPERC 8f.1.v1	CEPE SPERC 8f.1.v1 - CEPE 14 - Wide Dispersive Application of Decorative Coatings - Consumer and Professionals - outdoor use - Solids	0.0E+00	1.0E-02	5.0E-03	1.0E-02
30	CEPE SPERC 4.na.v1	CEPE SPERC 4.na.v1 - CEPE 15 - Other spray coating - Volatiles / Abatement	8.0E-01	2.0E-02	0.0E+00	8.2E-01
31	CEPE SPERC 4.nb.v1	CEPE SPERC 4.nb.v1 - CEPE 16a - Other spray coating, indoor use - point sources - Volatiles	9.8E-01	2.0E-02	0.0E+00	1.0E+00
32	CEPE SPERC 8a.n.v1	CEPE SPERC 8a.n.v1 - CEPE 16b - Other spray coating, indoor use - wide dispersive - Volatiles	9.8E-01	2.0E-02	0.0E+00	1.0E+00
33	CEPE SPERC 5.na.v1	CEPE SPERC 5.na.v1 - CEPE 17a - Other spray coating, indoor use - point sources - Solids	2.2E-02	0.0E+00	0.0E+00	2.2E-02
34	CEPE SPERC 8c.nb.v1	CEPE SPERC 8c.nb.v1 - CEPE 17b - Other spray coating, indoor use - wide dispersive - Solids	2.2E-02	0.0E+00	0.0E+00	2.2E-02
35	CEPE SPERC 5.na.v1	CEPE SPERC 5.na.v1 - CEPE 18 - Powder spraying	2.0E-02	0.0E+00	0.0E+00	2.0E-02
36	CEPE SPERC 8a.1a.v1	CEPE SPERC 8a.1a.v1 - CEPE 20 - application - consumer - bush/roller - indoor use - volatiles	9.9E-01	1.0E-02	0.0E+00	1.0E+00

37	CEPE SPERC 8c.1a.v1	CEPE SPERC 8c.1a.v1 - CEPE 21 - application - consumer - bush/roller - indoor use - solids	0.0E+00	1.0E-02	0.0E+00	1.0E-02
38	CEPE SPERC 8d.1a.v.1	CEPE SPERC 8d.1a.v.1 - CEPE 22 - application - consumer - bush/roller - outdoor use - volatiles	9.9E-01	1.0E-02	5.0E-03	1.0E+00
39	CEPE SPERC 8f.1a.v1	CEPE SPERC 8f.1a.v1 - CEPE 23 - application - consumer - bush/roller - outdoor use - solids	0.0E+00	1.0E-02	5.0E-03	1.0E-02
40	CEPE SPERC 8a.2a.v1	CEPE SPERC 8a.2a.v1 - CEPE 30 - application - professional - bush/roller - indoor use - volatiles	9.9E-01	1.0E-02	0.0E+00	1.0E+00
41	CEPE SPERC 8c.2a.v1	CEPE SPERC 8c.2a.v1 - CEPE 31 - application - professional - bush/roller - indoor use - solids	0.0E+00	1.0E-02	0.0E+00	1.0E-02
42	CEPE SPERC 8d.2a.v.1	CEPE SPERC 8d.2a.v.1 - CEPE 32 - application - professional - bush/roller - outdoor use - volatiles	9.9E-01	1.0E-02	5.0E-03	1.0E+00
43	CEPE SPERC 8f.2a.v1	CEPE SPERC 8f.2a.v1 - CEPE 33 - application - professional - bush/roller - outdoor use - solids	0.0E+00	1.0E-02	5.0E-03	1.0E-02
44	CEPE SPERC 8a.3a.v1	CEPE SPERC 8a.3a.v1 - CEPE 34 - application - professional - spraying - indoor use - volatiles	9.8E-01	2.0E-02	0.0E+00	1.0E+00
45	CEPE SPERC 8c.3a.v1	CEPE SPERC 8c.3a.v1 - CEPE 35 - application - professional - spraying - indoor use - solids	2.2E-02	0.0E+00	0.0E+00	2.2E-02
46	CEPE SPERC 8d.3a.v.1	CEPE SPERC 8d.3a.v.1 - CEPE 36 - application - professional - spraying - outdoor use - volatiles	9.8E-01	2.0E-02	0.0E+00	1.0E+00
47	CEPE SPERC 8f.3a.v1	CEPE SPERC 8f.3a.v1 - CEPE 37 - application - professional - spraying - outdoor use - solids	2.2E-02	0.0E+00		2.2E-02
48	CEPE SPERC 4.1a.v1	CEPE SPERC 4.1a.v1 - CEPE 50 - application - industrial - spraying - indoor use - incineration - volatiles	8.0E-03	2.0E-02	0.0E+00	2.8E-02
49	CEPE SPERC 4.1b.v1	CEPE SPERC 4.1b.v1 - CEPE 51 - application - industrial - spraying - indoor use - volatiles	9.8E-01	2.0E-02	0.0E+00	1.0E+00
50	CEPE SPERC 5.1a.v1	CEPE SPERC 5.1a.v1 - CEPE 52 - application - industrial - spraying - indoor use - solids	2.0E-02	0.0E+00	0.0E+00	2.0E-02
51	CEPE SPERC 5.2a.v1	CEPE SPERC 5.2a.v1 - CEPE 53 - application - industrial - spraying - indoor use - powder	2.0E-02	0.0E+00	0.0E+00	2.0E-02
52	ECCA SPERC 5.1a.v1	ECCA SPERC 5.1a.v1 - ECCA 1 - Industrial Coil Coating - Solids	0.0E+00	2.0E-03	0.0E+00	2.0E-03
53	ECCA SPERC 5.1b.v1	ECCA SPERC 5.1b.v1 - ECCA 2 - Industrial Coil Coating - Volatiles	1.2E-01	0.0E+00	0.0E+00	1.2E-01
54	EMPAC SPERC 5.1.v1	EMPAC SPERC 5.1.v1 - EMPAC 1 - Industrial Use of Paint, Coatings in metal packaging Non-Solvents	1.7E-02	0.0E+00	0.0E+00	1.7E-02
55	EMPAC SPERC 5.2.v1	EMPAC SPERC 5.2.v1 - EMPAC 2 - Industrial Use of Paint, Coatings in metal packaging Solvents	1.0E+00	0.0E+00	0.0E+00	1.0E+00
56	ACEA SPERC 5.1.v1	ACEA SPERC 5.1.v1 - ACEA 1 - Automotive vehicles - Solids	1.7E-02	0.0E+00	3.3E-01	1.7E-02
57	ACEA SPERC 4.1.v1	ACEA SPERC 4.1.v1 - ACEA 2 - Automotive vehicles - Volatiles/Solvents	7.5E-01	1.0E-02	0.0E+00	7.6E-01
58	AIRC SPERC 8c.1.v1	AIRC SPERC 8c.1.v1 - BFL_ZKF 1 - Vehicle Refinishing - Solids	2.5E-02	0.0E+00	4.8E-01	2.5E-02
59	AIRC SPERC 8a.1.v1	AIRC SPERC 8a.1.v1 - BFL_ZKF 2 - Vehicle Refinishing - Volatiles/Solvents	9.7E-01	3.0E-02	0.0E+00	1.0E+00
60	COLIPA SPERC 2.1.a.v1	COLIPA SPERC 2.1.a.v1 - COLIPA 1 - Formulation of low viscosiy liquids (Shampoo, hair conditioner, shower gel, foam bath) (large scale)	0.0E+00	1.0E-03	0.0E+00	1.0E-03
61	COLIPA SPERC 2.1.b.v1	COLIPA SPERC 2.1.b.v1 - COLIPA 2 - Formulation of low viscosiy liquids (Shampoo, hair conditioner, shower gel, foam bath) (medium scale)	0.0E+00	2.0E-03	0.0E+00	2.0E-03
62	COLIPA SPERC 2.1.c.v1	COLIPA SPERC 2.1.c.v1 - COLIPA 3 - Formulation of low viscosiy liquids (Shampoo, hair conditioner, shower gel, foam bath) (Small Scale)	0.0E+00	4.0E-03	0.0E+00	4.0E-03
63	COLIPA SPERC 2.1.d.v1	COLIPA SPERC 2.1.d.v1 - COLIPA 4 - Formulation of Fine Fragrances - Cleaning with Water (medium scale)	0.0E+00	1.5E-02	0.0E+00	1.5E-02
64	COLIPA SPERC 2.1.e.v1	COLIPA SPERC 2.1.e.v1 - COLIPA 5 - Formulation of Fine Fragrances - Cleaning with Water (small scale)	0.0E+00	3.0E-02	0.0E+00	3.0E-02
65	COLIPA SPERC 2.1.f.v1	COLIPA SPERC 2.1.f.v1 - COLIPA 6 - Formulation of Medium Viscosity Body Care Products (medium scale)	0.0E+00	1.0E-02	0.0E+00	1.0E-02
66	COLIPA SPERC 2.1.g.v1	COLIPA SPERC 2.1.g.v1 - COLIPA 7 - Formulation of Medium Viscosity Body Care Products (Small scale)	0.0E+00	2.0E-02	0.0E+00	2.0E-02
67	COLIPA SPERC 2.1.h.v1	COLIPA SPERC 2.1.h.v1 - COLIPA 8 - Formulation of Non-liquid Creams ((skin care, body care, Mascara, Solar oil, Maku-up Foundation) (large scale)	0.0E+00	1.0E-02	0.0E+00	1.0E-02
68	COLIPA SPERC 2.1.i.v1	COLIPA SPERC 2.1.i.v1 - COLIPA 9 - Formulation of Non-liquid Creams ((skin care, body care, Mascara, Solar oil, Maku-up Foundation) (medium scale)	0.0E+00	2.0E-02	0.0E+00	2.0E-02
69	COLIPA SPERC 2.1.j.v1	COLIPA SPERC 2.1.j.v1 - COLIPA 10 - Formulation of Non-liquid Creams ((skin care, body care, Mascara, Solar oil, Maku-up Foundation) (small scale)	0.0E+00	4.0E-02	0.0E+00	4.0E-02
73	COLIPA SPERC 2.3.a.v1	COLIPA SPERC 2.3.a.v1 - COLIPA 14 - Formulation of body care soap (large scale)	0.0E+00	5.0E-04	0.0E+00	5.0E-04
74	COLIPA SPERC 2.3.b.v1	COLIPA SPERC 2.3.b.v1 - COLIPA 15 - Formulation of body care soap (medium scale)	0.0E+00	1.0E-03	0.0E+00	1.0E-03
75	COLIPA SPERC 2.3.c.v1	COLIPA SPERC 2.3.c.v1 - COLIPA 16 - Formulation of body care soap (small scale)	0.0E+00	2.0E-03	0.0E+00	2.0E-03
76	COLIPA SPERC 8a.1.a.v1	COLIPA SPERC 8a.1.a.v1 - COLIPA 17 - Wide Dispersive Use in 'Down the Drain' products - hair and skin care products (Consumers and Professionals)	0.0E+00	1.0E+00	0.0E+00	1.0E+00
77	COLIPA SPERC 8a.1.b.v1	COLIPA SPERC 8a.1.b.v1 - COLIPA 18 - Wide Dispersive Use of Aerosol products for hair and skin care (Propellants)	1.0E+00	0.0E+00	0.0E+00	1.0E+00
78	COLIPA SPERC 8a.1.c.v1	COLIPA SPERC 8a.1.c.v1 - COLIPA 19 - Wide Dispersive Use of Aerosol products for hair and skin care (Non-Propellants)	0.0E+00	1.0E+00	0.0E+00	1.0E+00
79	EFCC SPERC 2.1a.v1	EFCC SPERC 2.1a.v1 - EFCC 1 - Volatile substances (main component) for the Formulation of Construction Chemicals. Only applicable for volatile substances. Main component as e.g. solvents usually been used in concentrations above 5%.	1.0E-02	5.0E-03	0.0E+00	1.5E-02
80	EFCC SPERC 2.1b.v1	EFCC SPERC 2.1b.v1 - EFCC2 - Volatile substances (additives) for the Formulation of Construction Chemicals. Only applicable for volatile substances. Additives usually been used in concentrations below 5%.	1.0E-02	5.0E-03	0.0E+00	1.5E-02

81	EFCC SPERC 2.1c.v1	EFCC SPERC 2.1c.v1 - EFCC 3 - Non-Volatile substances for the Formulation of Construction Chemicals. Only applicable for non-volatile substances.	0.0E+00	5.0E-03	0.0E+00	5.0E-03
82	EFCC SPERC 4.1a.v1	EFCC SPERC 4.1a.v1 - EFCC 4 - Industrial use of volatile substances (main components) in Construction Chemicals. Only applicable for volatile substances. Main component as e.g. solvents usually been used in concentrations above 5%.	9.9E-01	0.0E+00	0.0E+00	9.9E-01
83	EFCC SPERC 4.1b.v1	EFCC SPERC 4.1b.v1 - EFCC 5 -Industrial use of volatile substances (additives) in Construction Chemicals. Only applicable for volatile substances. Additives usually been used in concentrations below 5%.	9.9E-01	0.0E+00	0.0E+00	9.9E-01
84	EFCC SPERC 5.1a.v1	EFCC SPERC 5.1a.v1 - EFCC 6 -Industrial use of non-volatile substances in Construction Chemicals. Only applicable for non-volatile substances.	1.7E-02	0.0E+00	0.0E+00	1.7E-02
85	EFCC SPERC 8A.1a.v1	EFCC SPERC 8A.1a.v1 - EFCC 7 -Wide dispersive use of volatile substances in in Construction Chemicals, indoor. Only applicable for volatile substances.	9.8E-01	1.0E-02	0.0E+00	9.9E-01
86	EFCC SPERC 8C.1a.v1	EFCC SPERC 8C.1a.v1 - EFCC 8 -Wide dispersive use of non-volatile substances in Construction Chemicals, indoor. Only applicable for non-volatile substances.	0.0E+00	1.0E-02	0.0E+00	1.0E-02
87	EFCC SPERC 8D.1a.v1	EFCC SPERC 8D.1a.v1 - EFCC 9 -Wide dispersive use of volatile substances in Construction Chemicals, outdoor. Only applicable for volatile substances.	9.8E-01	1.0E-02	0.0E+00	9.9E-01
88	EFCC SPERC 8F.1a.v1	EFCC SPERC 8F.1a.v1 - EFCC 10 -Wide dispersive use of non-volatile substances in Construction Chemicals, outdoor. Only applicable for non-volatile substances.	0.0E+00	1.0E-02	3.7E-02	1.0E-02
89	ESVOC SpERC 1.1.v1	ESVOC SpERC 1.1.v1 - ESVOC 1 - Manufacture of the substance and subsequent recycling/ recovery, including material transfers, storage, and maintenance	1.0E-06	3.0E-03	1.0E-04	3.0E-03
90	ESVOC SpERC 6.1a.v1	ESVOC SpERC 6.1a.v1 - ESVOC 2 - Use as a isolated intermediate not under stricitly controlled conditions	0.0E+00	3.0E-03	1.0E-03	3.0E-03
91	ESVOC SpERC 1.1b.v1	ESVOC SpERC 1.1b.v1 - ESVOC 3 -Loading (including marine vessel/barge, rail car and IBC loading) and repacking (including drums and small packs), including losses during off-site storage (e.g. terminals)	1.0E-04	1.0E-05	1.0E-05	1.1E-04
92	ESVOC SpERC 2.2.v1	ESVOC SpERC 2.2.v1 - ESVOC 4 -Formulation & packing of mixtures in batch or continuous operations, including storage, materials transfers, large and small scale packing, and maintenance	2.5E-03	2.0E-03	1.0E-04	4.5E-03
93	ESVOC SpERC 4.3a.v1	ESVOC SpERC 4.3a.v1 - ESVOC 5 -Covers the use in coatings (paints, inks, adhesives, etc) including exposures during use (including materials transfer from bulk and semi-bulk and spraying, brushing and other manual application tasks); and equipment cleaning	9.8E-01	7.0E-03	0.0E+00	9.9E-01
94	ESVOC SpERC 8.3b.v1	ESVOC SpERC 8.3b.v1 - ESVOC 6 -Covers the use in coatings (paints, inks, adhesives, etc) including exposures during use (including materials transfer and spraying, brushing and other manual application tasks); and equipment cleaning	9.8E-01	1.0E-02	1.0E-02	9.9E-01
95	ESVOC SpERC 8.3c.v1	ESVOC SpERC 8.3c.v1 - ESVOC 7 -Covers the use in coatings (paints, inks, adhesives, etc) including exposures during use (including product transfer and spraying, brushing, aerosol and other manual application tasks); and equipment cleaning	9.9E-01	1.0E-02	5.0E-03	1.0E+00
96	ESVOC SpERC 4.4a.v1	ESVOC SpERC 4.4a.v1 - ESVOC 8 -Covers the use as a component of cleaning products for industrial use including transfer from storage; pouring/unloading from drums or containers; exposures during cleaning activities (automated and by hand); and related maintenance	3.0E-01	3.0E-05	0.0E+00	3.0E-01
97	ESVOC SpERC 8.4b.v1	ESVOC SpERC 8.4b.v1 - ESVOC 9 -Covers the use as a component of cleaning products for professional use including pouring/unloading from drums or containers; and exposures during cleaning activities (automated and by hand)	2.0E-02	1.0E-06	0.0E+00	2.0E-02
98	ESVOC SpERC 8.4c.v1	ESVOC SpERC 8.4c.v1 - ESVOC 10 -Covers general exposures to consumers arising from the use household products sold as washing and cleaning products, aerosols, coatings, de-icers, lubricants and air care products	9.5E-01	2.5E-02	2.5E-02	9.8E-01
99	ESVOC SpERC 4.6a.v1	ESVOC SpERC 4.6a.v1 - ESVOC 13 - Covers the industrial use of formulated lubricants in closed and open systems including transfer operations, operation of engines and similar articles, maintenance and disposal of waste oil	3.0E-05	3.0E-04	1.0E-03	3.3E-04
100	ESVOC SpERC 9.6b.v1	ESVOC SpERC 9.6b.v1 - ESVOC 14 - Covers the professional use of formulated lubricants in closed systems including transfer operations, operation of engines and similar articles, recycling and disposal of waste oil	1.0E-02	1.0E-02	1.0E-02	2.0E-02
101	ESVOC SpERC 8.6c.v1	ESVOC SpERC 8.6c.v1 - ESVOC 15 - Covers the professional use of formulated lubricants in open systems including transfer operations, operation of engines and similar articles, recycling and disposal of waste oil	5.0E-03	5.0E-02	5.0E-02	5.5E-02
102	ESVOC SpERC 9.6d.v1	ESVOC SpERC 9.6d.v1 - ESVOC 16 - Covers the consumer use of formulated lubricants in closed systems including transfer operations, application, operation of engines and similar articles, recycling and disposal of waste oil.	1.0E-02	1.0E-02	1.0E-02	2.0E-02
103	ESVOC SpERC 8.6e.v1	ESVOC SpERC 8.6e.v1 - ESVOC 17 - Covers the consumer use of formulated lubricants in open systems including transfer operations, application, operation of engines and similar articles, recycling and disposal of waste oil.	5.0E-03	5.0E-02	5.0E-02	5.5E-02
104	ESVOC SpERC 4.7a.v1	ESVOC SpERC 4.7a.v1 - ESVOC 18 - Covers the industrial use in formulated MWFs/rolling oils including transfer operations, open rolling and annealing activities, open and contained cutting/machining activities, draining and working on contaminated/ reject articles, recycling and disposal of waste oils.	6.0E-03	3.0E-04	0.0E+00	6.3E-03
105	ESVOC SpERC 8.7c.v1	ESVOC SpERC 8.7c.v1 - ESVOC 20 - Covers the professional use in formulated MWFs/rolling oils including transfer operations, open rolling and annealing activities, open and contained cutting/machining activities, draining and working on contaminated/ reject articles, recycling and disposal of waste oils.	5.0E-03	5.0E-02	5.0E-02	5.5E-02

106	ESVOC SpERC 4.9.v1	ESVOC SpERC 4.9.v1 - ESVOC 23 - Use as a blowing agent, including material transfers, curing, storage and maintenance	1.0E+00	3.0E-04	0.0E+00	1.0E+00
107	ESVOC SpERC 4.10a.v1	ESVOC SpERC 4.10a.v1 - ESVOC 24 - Use as binders and release agents in industrial settings, including material transfers, mixing, application and disposal	2.0E-01	3.0E-05	0.0E+00	2.0E-01
108	ESVOC SpERC 8.10b.v1	ESVOC SpERC 8.10b.v1 - ESVOC 25 - Use as binders and release agents in professional settings, including material transfers, mixing, application and disposal	9.5E-01	2.5E-02	2.5E-02	9.8E-01
109	ESVOC SpERC 8.11a.v1	ESVOC SpERC 8.11a.v1 - ESVOC 26 - Use as an agrochemical excipient for application by manual or machine spraying, smokes and fogging.	9.0E-01	1.0E-02	9.0E-02	9.1E-01
110	ESVOC SpERC 8.11b.v1	ESVOC SpERC 8.11b.v1 - ESVOC 27 - Use as an agrochemical excipient for application by manual spraying and aerosols	9.0E-01	1.0E-02	9.0E-02	9.1E-01
111	ESVOC SpERC 7.12a.v1	ESVOC SpERC 7.12a.v1 - ESVOC 28 - Use as a fuel including incineration of wastes and use as a solvent in fuel additives, covers refueling and evaporative losses	2.5E-04	1.0E-05	0.0E+00	2.6E-04
112	ESVOC SpERC 9.12b.v1	ESVOC SpERC 9.12b.v1 - ESVOC 29 - Use as a fuel including use as a solvent in fuel additives; covers refueling and evaporative losses	1.0E-04	1.0E-05	1.0E-05	1.1E-04
113	ESVOC SpERC 9.12c.v1	ESVOC SpERC 9.12c.v1 - ESVOC 30 - Use as a fuel including use as a solvent in fuel additives, covers refueling and evaporative losses	1.0E-04	1.0E-05	1.0E-05	1.1E-04
114	ESVOC SpERC 7.13a.v1	ESVOC SpERC 7.13a.v1 - ESVOC 31 - Use as functional fluids e.g. cable oils, transfer oils, insulators, hydraulic fluids in industrial equipment including maintenance and related material transfers	1.0E-04	3.0E-04	1.0E-03	4.0E-04
115	ESVOC SpERC 9.13b.v1	ESVOC SpERC 9.13b.v1 - ESVOC 32 - Use as functional fluids e.g. cable oils, transfer oils, insulators, hydraulic fluids in professional equipment including maintenance	5.0E-02	2.5E-02	2.5E-02	7.5E-02
116	ESVOC SpERC 9.13c.v1	ESVOC SpERC 9.13c.v1 - ESVOC 33 - Use of sealed items containing functional fluids e.g. transfer oils, hydraulic fluids	5.0E-02	2.5E-02	2.5E-02	7.5E-02
117	ESVOC SpERC 8.14a.v1	ESVOC SpERC 8.14a.v1 - ESVOC 34 - De-icing of vehicles, aircraft and other equipment by spraying	9.5E-01	1.0E-02	4.0E-02	9.6E-01
118	ESVOC SpERC 8.14b.v1	ESVOC SpERC 8.14b.v1 - ESVOC 35 - De-icing of vehicles and similar equipment by spraying	9.0E-01	5.0E-02	5.0E-02	9.5E-01
119	ESVOC SpERC 8.15.v1	ESVOC SpERC 8.15.v1 - ESVOC 36 - Application of surface coatings and binders in road and construction activities, including material transfers and procut disposal	9.5E-01	1.0E-02	4.0E-02	9.6E-01
120	ESVOC SpERC 8.16.v1	ESVOC SpERC 8.16.v1 - ESVOC 37 - Other Consumer Uses: Consumer	9.5E-01	2.5E-02	2.5E-02	9.8E-01
121	ESVOC SPERC 4.24.v1	ESVOC SPERC 4.24.v1 - ESVOC 38 - Use of the substance within laboratory setting, including pilot plants	2.5E-02	2.0E-02	1.0E-04	4.5E-02
122	ESVOC SpERC 8.17.v1	ESVOC SpERC 8.17.v1 - ESVOC 39 - Use of small quantities within laboratory settings	5.0E-01	5.0E-01	0.0E+00	1.0E+00
123	ESVOC SpERC 2.18.v1	ESVOC SpERC 2.18.v1 - ESVOC 40 - Covers exposures arising from the manufacture of slurry explosives (including materials transfer, mixing and charging) and equipment cleaning	1.0E-04	3.0E-04	1.0E-04	4.0E-04
124	ESVOC SPERC 8.24.v1	ESVOC SPERC 8.24.v1 - ESVOC 41 - Explosives manufacture: Professional	1.0E-03	2.0E-02	1.0E-02	2.1E-02
125	ESVOC SpERC 4.19.v1	ESVOC SpERC 4.19.v1 - ESVOC 42 - Manufacture of rubber articles, including processing of raw rubber, handling and mixing of rubber additives, vulcanising, cooling and finishing.	1.0E-02	3.0E-03	1.0E-04	1.3E-02
126	ESVOC SpERC 4.20.v1	ESVOC SpERC 4.20.v1 - ESVOC 43 - Manufacture of polymers from monomers in continuous and batch processes, include sparging, discharging, and reactor maintenance and immediate polymer product formation (i.e. compounding, pelletisation, product off-gassing).	2.0E-03	3.0E-03	1.0E-04	5.0E-03
127	ESVOC SpERC 4.21a.v1	ESVOC SpERC 4.21a.v1 - ESVOC 44 - Processing of formulated polymers including material transfers, additives handling, moulding, curing and forming activities, material re-works and associated maintenance.	2.0E-02	0.0E+00	1.0E-05	2.0E-02
128	ESVOC SpERC 8.21b.v1	ESVOC SpERC 8.21b.v1 - ESVOC 45 - Processing of formulated polymers including material transfers, moulding and forming activities, material re-works and associated maintenance.	9.8E-01	1.0E-02	1.0E-02	9.9E-01
129	ESVOC SpERC 3.22a.v1	ESVOC SpERC 3.22a.v1 - ESVOC 46 - Covers the use of the substance for the treatment of water at industrial facilities in open and closed systems	5.0E-02	9.5E-01	0.0E+00	1.0E+00
130	ESVOC SpERC 8.22b.v1	ESVOC SpERC 8.22b.v1 - ESVOC 47 - Covers the use of the substance for the treatment of water in open and closed systems	1.0E-02	9.9E-01	0.0E+00	1.0E+00
131	ESVOC SpERC 8.22c.v1	ESVOC SpERC 8.22c.v1 - ESVOC 48 - Covers the use of the substance for the treatment of water in open and closed systems	1.0E-02	9.9E-01	0.0E+00	1.0E+00
132	ESVOC SpERC 4.23.v1	ESVOC SpERC 4.23.v1 - ESVOC 49 - Covers the use of the substance in extraction processes at mining operations, including material transfers, winning and separation activities, and substance recovery and disposal.	5.0E-02	5.0E-01	5.0E-02	5.5E-01
133	ESVOC SpERC 9.24a.v1	ESVOC SpERC 9.24a.v1 - ESVOC 50 - Release of unburned residual fuel in exhaust from combusiton of fuel in stationary enginges, e.g. industrial fuel combustion	1.0E-03	0.0E+00	0.0E+00	1.0E-03
134	ESVOC SpERC 9.24b.v1	ESVOC SpERC 9.24b.v1 - ESVOC 51 - Release of unburned residual fuel in exhaust from combusiton of fuel in stationary enginges, e.g. heating oil	5.0E-03	0.0E+00	0.0E+00	5.0E-03
135	ESVOC SpERC 9.24c.v1	ESVOC SpERC 9.24c.v1 - ESVOC 52 - Release of unburned residual fuel in exhaust from combusiton of fuel in stationary enginges, e.g. heating oil	5.0E-03	0.0E+00	0.0E+00	5.0E-03
136	FEICA SPERC 2.1a.v1	FEICA SPERC 2.1a.v1 - FEICA 1 - Formulation of Solventless/ Solvent Borne Adhesives - Solids	1.0E-02	5.0E-05	0.0E+00	1.0E-02
137	FEICA SPERC 2.1b.v1	FEICA SPERC 2.1b.v1 - FEICA 2 - Formulation of Solvent Borne adhesives - Volatiles (Large Scale)	1.2E-03	0.0E+00	0.0E+00	1.2E-03
138	FEICA SPERC 2.1c.v1	FEICA SPERC 2.1c.v1 - FEICA 3 - Formulation of Solvent Borne adhesives - Volatiles (Small Scale)	6.0E-03	0.0E+00	0.0E+00	6.0E-03

139	FEICA SPERC 2.2a.v1	FEICA SPERC 2.2a.v1 - FEICA 4 - Formulation of Water Borne adhesives - Volatiles	4.0E-03	5.0E-02	0.0E+00	5.4E-02
140	FEICA SPERC 2.2b.v1	FEICA SPERC 2.2b.v1 - FEICA 5 - Formulation of Water Borne adhesives - Solids	9.7E-05	5.0E-02	0.0E+00	5.0E-02
141	FEICA SPERC 5.1a.v1	FEICA SPERC 5.1a.v1 - FEICA 6 - Industrial Use of Substances other than Solvents in Paper, Board and related Products / Woodworking and joinery / Footwear and Leather, Textile, Others Adhesives	9.0E-03	0.0E+00	0.0E+00	9.0E-03
142	FEICA SPERC 5.1b.v1	FEICA SPERC 5.1b.v1 - FEICA 7 - Industrial Use of Substances other than Solvents in Transportation (Automotive/aircraft/rail vehicles) / industrial Building Construction Adhesives	1.7E-02	0.0E+00	0.0E+00	1.7E-02
143	FEICA SPERC 5.2a.v1	FEICA SPERC 5.2a.v1 - FEICA 8 - Industrial Use of Solvents in Paper, Board and related Products / Woodworking and joinery / Footwear and Leather, Textile, Others Adhesives	9.9E-01	0.0E+00	0.0E+00	9.9E-01
144	FEICA SPERC 5.2b.v1	FEICA SPERC 5.2b.v1 - FEICA 9 - Industrial Use of Solvents in Transportation (Automotive/aircraft/rail vehicles) / industrial Building Construction Adhesives	9.9E-01	0.0E+00	0.0E+00	9.9E-01
145	FEICA SPERC 8c.1a.v1	FEICA SPERC 8c.1a.v1 - FEICA 10 - Wide dispersive Use of Substances other than Solvents in Building Construction Adhesives for indoor application	0.0E+00	1.0E-02	0.0E+00	1.0E-02
146	FEICA SPERC 8c.1b.v1	FEICA SPERC 8c.1b.v1 - FEICA 11 - Wide dispersive Use of Substances other than Solvents in Professional and DIY Adhesives	0.0E+00	9.0E-03	0.0E+00	9.0E-03
147	FEICA SPERC 8a.2a.v1	FEICA SPERC 8a.2a.v1 - FEICA 12 - Wide dispersive Use of Solvents in Building Construction Adhesives for indoor application	9.8E-01	1.0E-02	0.0E+00	9.9E-01
148	FEICA SPERC 8a.2b.v1	FEICA SPERC 8a.2b.v1 - FEICA 13 - Wide dispersive Use of Solvents in Professional and DIY Adhesives	9.9E-01	0.0E+00	0.0E+00	9.9E-01
149	FEICA SPERC 8f.1.v1	FEICA SPERC 8f.1.v1 - FEICA 14 - Wide dispersive Use of Substances other than Solvents in Building Construction Adhesives for outdoor application	0.0E+00	1.0E-02	0.0E+00	1.0E-02
150	FEICA SPERC 8d.2.v1	FEICA SPERC 8d.2.v1 - FEICA 15 - Wide dispersive Use of Solvents in Building Construction Adhesives for outdoor application	9.8E-01	1.0E-02	0.0E+00	9.9E-01
151	ECPA SPERC 8d.1.v1	ECPA SPERC 8d.1.v1 - ECPA 1 - Direct application of granules or treated seeds to soil	0.0E+00	0.0E+00	1.0E+00	0.0E+00
152	ECPA SPERC 8d.2.v2	ECPA SPERC 8d.2.v2 - ECPA 2 - Spray application of plant protection products (releases dependent on co-formulant vapour pressure)	1.0E-02	0.0E+00	9.9E-01	1.0E-02
153	ETRMA SPERC 3/6d.1a v.2	ETRMA SPERC 3/6d.1a v.2 - ETRMA 3/6d.1a - Process with efficient raw material use - GRG use of vulcanization agents, anti-ageing agents / antidegradants	1.0E-03	2.0E-04	0.0E+00	1.2E-03
154	ETRMA SPERC 3/6d.1b v.2	ETRMA SPERC 3/6d.1b v.2 - ETRMA 3/6d.1b - Process with efficient raw material use - GRG use of reinforcing agents, hardeners	1.0E-03	2.0E-04	0.0E+00	1.2E-03
155	ETRMA SPERC 3/6d.1c v.2	ETRMA SPERC 3/6d.1c v.2 - ETRMA 3/6d.1c - Process with efficient raw material use - GRG use of bonding agents	1.0E-03	2.0E-04	0.0E+00	1.2E-03
156	ETRMA SPERC 3/6d.1d v.2	ETRMA SPERC 3/6d.1d v.2 - ETRMA 3/6d.1d - Process with efficient raw material use - GRG use of mastication agents/peptiser	1.0E-03	2.0E-04	0.0E+00	1.2E-03
157	ETRMA SPERC 3/6d.2a v.2	ETRMA SPERC 3/6d.2a v.2 - ETRMA 3/6d.2a - Process with efficient raw material use and mechanical pre-treatment - GRG use of vulcanization agents, anti-ageing agents / antidegradants	1.0E-03	8.0E-05	0.0E+00	1.1E-03
158	ETRMA SPERC 3/6d.2b v.2	ETRMA SPERC 3/6d.2b v.2 - ETRMA 3/6d.2b - Process with efficient raw material use and mechanical pre-treatment - GRG use of reinforcing agents, hardeners	1.0E-03	8.0E-05	0.0E+00	1.1E-03
159	ETRMA SPERC 3/6d.2c v.2	ETRMA SPERC 3/6d.2c v.2 - ETRMA 3/6d.2c - Process with efficient raw material use and mechanical pre-treatment - GRG use of bonding agents	1.0E-03	8.0E-05	0.0E+00	1.1E-03
160	ETRMA SPERC 3/6d.2d v.2	ETRMA SPERC 3/6d.2d v.2 - ETRMA 3/6d.2d - Process with efficient raw material use and mechanical pre-treatment - GRG use of mastication agents/peptiser	1.0E-03	8.0E-05	0.0E+00	1.1E-03
161	ETRMA SPERC 3/6d.3a v.1	ETRMA SPERC 3/6d.3a v.1 - ETRMA 3/6d.3a - Process with optimization for efficient raw materials use - Tyre use of reinforcing agents, hardeners, mastication agents/peptiser, anti-aging agents/antidegradants and GRG use of tackifiers, filler activators and bonding agents.	1.0E-03	1.0E-05	0.0E+00	1.0E-03
162	ETRMA SPERC 3/6d.3b v.1	ETRMA SPERC 3/6d.3b v.1 - ETRMA 3/6d.3b - Process with optimization for efficient raw materials use - Tyre use of vulcanization agents, lubricants, tackifiers, filler activators, bonding agents and GRG use of fillers and pigments.	1.0E-03	1.0E-05	0.0E+00	1.0E-03
163	ETRMA SPERC 3/6d.3c v.1	ETRMA SPERC 3/6d.3c v.1 - ETRMA 3/6d.3c - Process with optimization for efficient raw materials use - Tyre use of fillers and pigments.	1.0E-03	1.0E-05	0.0E+00	1.0E-03
164	TEGEWA SPERC 5.1a.v1	TEGEWA SPERC 5.1a.v1 - TEGEWA 1 - Dyeing of Textiles - High efficiency	0.0E+00	5.0E-02	0.0E+00	5.0E-02
165	TEGEWA SPERC 5.1b.v1	TEGEWA SPERC 5.1b.v1 - TEGEWA 2 - Dyeing of Textiles - Normal efficiency	0.0E+00	3.0E-01	0.0E+00	3.0E-01
166	TEGEWA SPERC 5.1c.v1	TEGEWA SPERC 5.1c.v1 - TEGEWA 3 - Textile Finishing and Coating - Residues not retained	1.0E-03	2.0E-01	0.0E+00	2.0E-01
167	TEGEWA SPERC 5.1d.v1	TEGEWA SPERC 5.1d.v1 - TEGEWA 4 - Textile Finishing and Coating - Residues retained	0.0E+00	5.0E-02	0.0E+00	5.0E-02
168	TEGEWA SPERC 6b.1.v1	TEGEWA SPERC 6b.1.v1 - TEGEWA 5 - Use of reactive processing aid in textile processing	0.0E+00	2.0E-02	0.0E+00	2.0E-02
169	TEGEWA SPERC 4.1.v1	TEGEWA SPERC 4.1.v1 - TEGEWA 6 - Industrial Use of Water Borne Processing Aids - no RMM	0.0E+00	1.0E+00	0.0E+00	1.0E+00
70	COLIPA SPERC 2.2.a.v1	COLIPA SPERC 2.2.a.v1 - COLIPA 11 - Formulation of cosmetic products involving cleaning with Organic Solvents (Varnish / Removers, Decorative Cosmetics, Spray, Lacquer, Fine Fragrance, Solar oil, solid products - (large scale)	0.0E+00	0.0E+00	0.0E+00	0.0E+00
71	COLIPA SPERC 2.2.b.v1	COLIPA SPERC 2.2.b.v1 - COLIPA 12 - Formulation of cosmetic products involving cleaning with Organic Solvents (Varnish / Removers, Decorative Cosmetics, Spray, Lacquer, Fine Fragrance, Solar oil, solid products - (medium scale)	0.0E+00	0.0E+00	0.0E+00	0.0E+00
72	COLIPA SPERC 2.2.c.v1	COLIPA SPERC 2.2.c.v1 - COLIPA 13- Formulation of cosmetic products involving cleaning with Organic Solvents (Varnish / Removers, Decorative Cosmetics, Spray, Lacquer, Fine Fragrance, Solar oil, solid products - (small scale)	0.0E+00	0.0E+00	0.0E+00	0.0E+00

Table SI-2.

See: Table SI-2.pdf

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
REACH - mono constituent organic substances																							
count							*3939*	*3939*	*3735*	*3716*	*3735*	*1256*	*962*	*3322*	*3322*	*3322*	*3940*	*1489*	*3917*	*3917*	*3909*	*3909*	*3909*
sum or mean																	*2.7E+08*	*1.6E+08*	*4.9E+07*	*19%*			
standard deviation																					*1.4*	*1.3*	*1.5*
2.5-p																	*1.5E+00*	*2.7E+00*	*2.6E-01*	*14%*	*-11.1*	*-11.3*	*-13.3*
50-p							*204*	*36*	*2.5E-02*	*2.6E+02*	*1.0E+02*	*9.2*	*7.0*	*1.1E-06*	*1.1E-07*	*3.5E-07*	*7.1E+02*	*8.5E+02*	*1.2E+02*	*16%*	*-8.6*	*-8.7*	*-10.5*
97.5-p																	*2.4E+05*	*8.2E+05*	*4.5E+04*	*24%*	*-5.8*	*-6.1*	*-7.5*
urea	200-315-5	57-13-6	57136	719	Reach_39	1	60	29.0	2.8E+01	4.2E+05	2.8E-02	14.3	14	7.0E-07	3.5E-07	1.1E-06				15%	-3.7	-3.8	-5.8
α,α-dimethylbenzyl hydroperoxide	201-254-7	80-15-9	80159	932	Reach_259	2	152	38.7	9.3E+00	7.3E+04	1.4E+02	12.3		1.2E-08	3.5E-08	1.1E-07				23%	-4.1	-3.9	-4.9
ε-caprolactam	203-313-2	105-60-2	105602	180	Reach_646	3	113	66.7	4.8E-01	3.7E+04	4.6E+00	15.1	14	2.4E-07	3.5E-07	1.1E-06				17%	-4.2	-4.4	-6.1
4,4'-isopropylidenediphenol	201-245-8	80-05-7	80057	96	Reach_254	4	228	131.8	3.0E-05	3.7E+02	4.4E+03	9.7		1.3E-07	3.5E-08	1.1E-07				19%	-4.0	-4.5	-6.1
adipic acid, compound with hexane-1,6-diamine (1:1)	222-037-3	3323-53-3	3323533	5845	Reach_1947	5	262	0.0												18%	-4.2	-4.5	-6.2
terephthalic acid	202-830-0	100-21-0	100210	122	Reach_552	6	166	126.6	1.6E-03	2.8E+03	5.8E+01	3.5		9.4E-07	3.5E-07	1.1E-06				15%	-4.0	-4.6	-6.5
melamine	203-615-4	108-78-1	108781	4	Reach_756	7	126	133.1	1.2E-05	9.1E+05	4.2E-01		8.7	1.6E-07	1.1E-07	1.1E-07				18%	-3.6	-4.6	-6.3
4,4'-Isopropylidenediphenol, oligomeric reaction products with	500-033-5	25068-38-6	25068386	5795	Reach_4051	8	321	0.0												18%	-4.5	-4.8	-6.5
2,2',2''-nitrilotriethanol	203-049-8	102-71-6	102716	155	Reach_596	9	149	83.3	4.5E-04	1.0E+06	3.3E-03	14.5	6	6.7E-09	1.1E-06	3.5E-06				23%	-4.3	-4.9	-5.9
aniline	200-539-3	62-53-3	62533	765	Reach_64	10	93	-6.2	1.1E+02	1.7E+04	1.2E+01		9	4.3E-07	1.1E-07	1.1E-06				16%	-4.9	-4.9	-6.7
sodium acrylate	231-209-7	7446-81-3	7446813	6021	Reach_2250	11	94	0.0												18%	-4.6	-4.9	-6.6
phenol	203-632-7	108-95-2	108952	252	Reach_765	12	94	-2.3	4.3E+01	3.5E+04	3.2E+01	10		9.3E-07	3.5E-07	1.1E-06				15%	-5.2	-4.9	-6.7
methanol	200-659-6	67-56-1	67561	793	Reach_84	13	32	-101.0	1.6E+04	8.0E+05	2.3E-01	15.9		4.7E-06	1.1E-06	3.5E-06				14%	-5.3	-5.1	-6.7
2-aminoethanol	205-483-3	141-43-5	141435	456	Reach_1162	14	61	-27.6	5.5E+01	1.0E+06	2.5E-02	15	5	4.1E-07	1.1E-06	3.5E-06				16%	-5.1	-5.1	-7.0
pentaerythritol	204-104-9	115-77-5	115775	341	Reach_944	15	136	88.7	3.4E-06	1.0E+06	1.7E-02	14.4		3.9E-08	3.5E-07	1.1E-06				21%	-4.3	-5.1	-6.4
propane-1,2-diol	200-338-0	57-55-6	57556	722	Reach_41	16	76	-33.0	1.5E+01	1.7E+06	1.7E-01	14.9		5.5E-07	3.5E-07	1.1E-06				15%	-4.7	-5.2	-7.1
ethanol	200-578-6	64-17-5	64175	776	Reach_70	17	46	-87.8	8.1E+03	6.3E+05	7.2E-01	15.9		4.3E-06	1.1E-06	3.5E-06				14%	-5.4	-5.2	-6.8
but-2-yne-1,4-diol	203-788-6	110-65-6	110656	281	Reach_824	18	86	29.0	3.3E-01	1.8E+05	1.2E-01	13.2		1.7E-07	1.1E-06	3.5E-06				18%	-4.7	-5.2	-6.8
ethylene	200-815-3	74-85-1	74851	3647	Reach_111	3	28	-150.9	4.2E+06	3.6E+03	1.9E+01			1.1E-06	1.1E-07	3.5E-07				20%	-5.6	-5.2	-7.9
calcium cyanamide	205-861-8	156-62-7	156627	5721	Reach_1215	4	80	0.0												18%	-5.0	-5.3	-6.9
propylidynetrimethanol	201-074-9	77-99-6	77996	890	Reach_192	5	134	59.7	5.6E-03	1.9E+05	1.5E+00	14.8		3.0E-08	1.1E-06	3.5E-06				22%	-4.9	-5.3	-6.5
benzene	200-753-7	71-43-2	71432	821	Reach_103	6	78	-77.9	1.2E+04	1.1E+03	9.8E+01			2.2E-08	3.5E-08	1.1E-07				23%	-5.7	-5.3	-7.8
[2-(acryloyloxy)ethyl]trimethylammonium chloride	256-176-6	44992-01-0	44992010	5888	Reach_2756	7	194	0.0												18%	-5.0	-5.3	-7.0
sodium methanolate	204-699-5	124-41-4	124414	5636	Reach_1078	8	54	0.0												18%	-5.0	-5.3	-7.0
acrylamide	201-173-7	79-06-1	79061	911	Reach_226	9	71	21.7	1.7E+01	9.4E+05	1.5E-01	15.1	14	3.5E-07	3.5E-07	1.1E-06				16%	-5.1	-5.4	-7.2
etidronic acid	220-552-8	2809-21-4	2809214	578	Reach_1871	10	206	88.0	1.7E-08	1.0E+06	9.8E-01	1.9		8.4E-09	3.5E-07	1.1E-06				23%	-4.7	-5.4	-6.4
cyanuric acid	203-618-0	108-80-5	108805	245	Reach_757	11	129	120.4	3.2E-03	1.7E+05	4.1E+00	6.8		2.2E-09	1.1E-07	3.5E-07				23%	-4.8	-5.4	-6.3
1,2-dichloroethane	203-458-1	107-06-2	107062	206	Reach_691	12	99	-76.8	1.0E+04	9.9E+03	6.8E+01			1.4E-08	3.5E-08	1.1E-07				23%	-5.7	-5.4	-7.4
adipic acid	204-673-3	124-04-9	124049	400	Reach_1065	13	146	102.0	1.7E-03	6.5E+04	1.7E+00	4.51		1.2E-06	3.5E-07	1.1E-06				14%	-4.4	-5.4	-7.3
tert-butyl methyl ether	216-653-1	1634-04-4	1634044	33	Reach_1701	14	88	-94.3	3.4E+04	5.9E+04	2.7E+01			4.6E-09	1.1E-07	3.5E-07				23%	-5.7	-5.4	-7.2
oxydipropanol	246-770-3	25265-71-8	25265718	566	Reach_2562	15	134	30.9	2.0E-01	2.3E+06	3.2E-01	15.2		9.2E-08	1.1E-07	3.5E-07				19%	-4.6	-5.4	-6.9
trisodium citrate	200-675-3	68-04-2	68042	1232	Reach_89	16	258	0.0												18%	-5.1	-5.4	-7.1
propene	204-062-1	115-07-1	115071	1629	Reach_935	17	42	-135.4	9.4E+05	2.1E+03	4.8E+01			1.1E-06	1.1E-07	3.5E-07				20%	-5.8	-5.4	-8.3
calcium tartrate	221-621-5	3164-34-9	3164349	5841	Reach_1923	18	188	0.0												18%	-5.1	-5.4	-7.1
2,2'-iminodi(ethylamine)	203-865-4	111-40-0	111400	299	Reach_854	19	103	17.8	3.4E+01	1.0E+06	7.4E-03		4	2.9E-09	1.1E-06	3.5E-06				23%	-5.6	-5.5	-6.4
2-methylpropan-2-ol	200-889-7	75-65-0	75650	863	Reach_156	20	74	-73.8	6.3E+03	2.0E+05	5.4E+00	16		4.6E-08	3.5E-07	1.1E-06				21%	-5.8	-5.5	-6.7
ethane-1,2-diol	203-473-3	107-21-1	107211	216	Reach_700	21	62	-31.6	8.1E+00	7.3E+05	6.3E-02	14.8		4.4E-06	1.1E-06	3.5E-06				14%	-5.0	-5.5	-7.5
tetrasodium ethylenediaminetetraacetate	200-573-9	64-02-8	64028	1229	Reach_68	22	380	0.0												18%	-5.2	-5.5	-7.2
calcium diformate	208-863-7	544-17-2	544172	5925	Reach_1353	23	130	0.0												18%	-5.3	-5.6	-7.2
phthalic anhydride	201-607-5	85-44-9	85449	966	Reach_297	24	148	21.8	3.0E-02	5.3E+02	1.2E+02			1.2E-06	1.1E-07	3.5E-07				14%	-5.7	-5.6	-7.5
2,2'-iminodiethanol	203-868-0	111-42-2	111422	300	Reach_856	25	105	28.8	7.2E-02	3.2E+05	1.9E-02	14.7	5	5.0E-07	1.1E-06	3.5E-06				15%	-4.8	-5.6	-7.5
trimethylammonium chloride	209-810-0	593-81-7	593817	1227	Reach_1396	26	96	0.0												18%	-5.3	-5.6	-7.3
citric acid	201-069-1	77-92-9	77929	889	Reach_189	27	192	169.2	7.5E-07	2.4E+05	2.1E-02	2.97		8.4E-07	3.5E-07	1.1E-06				15%	-4.4	-5.6	-7.6
chloroethylene	200-831-0	75-01-4	75014	845	Reach_123	28	62	-122.0	3.6E+05	4.8E+03	4.2E+01			9.7E-09	3.5E-08	1.1E-07				24%	-6.1	-5.6	-8.2
1-phenylethanol	202-707-1	98-85-1	98851	4194	Reach_520	29	122	-6.9	7.3E+00	1.1E+04	3.1E+01	14.9		1.1E-06	1.1E-07	3.5E-07				14%	-5.9	-5.7	-7.5
4-methyl-m-phenylene diisocyanate	209-544-5	584-84-9	584849	729	Reach_1384	30	174	19.2	3.4E+00	1.3E+03	5.5E+03			4.5E-08	1.1E-07	3.5E-07				21%	-5.9	-5.7	-6.9
diphenyl carbonate	203-005-8	102-09-0	102090	1336	Reach_590	31	214	-2.1	5.3E-02	4.5E+01	1.6E+03			3.5E-07	1.1E-07	3.5E-07				16%	-5.9	-5.7	-7.4
styrene	202-851-5	100-42-5	100425	125	Reach_557	32	104	-48.3	6.7E+02	2.9E+02	7.8E+02			7.3E-07	3.5E-08	1.1E-07				18%	-6.0	-5.7	-7.9
hexamethylenediamine	204-679-6	124-09-4	124094	1783	Reach_1067	33	116	24.5	2.4E+01	1.1E+06	2.2E+00		3.23	1.1E-06	3.5E-07	1.1E-06				14%	-5.6	-5.7	-7.7
maleic anhydride	203-571-6	108-31-6	108316	235	Reach_740	34	98	-51.6	2.2E+01	9.7E+04	4.2E+01			6.4E-07	3.5E-07	1.1E-06				15%	-5.9	-5.7	-7.5
acetic acid	200-580-7	64-19-7	64197	778	Reach_72	35	60	-21.3	2.3E+03	9.6E+05	1.2E+00	4.9		4.7E-06	3.5E-07	3.5E-07				14%	-5.0	-5.7	-7.8
(3-chloro-2-hydroxypropyl)trimethylammonium chloride	222-048-3	3327-22-8	3327228	5846	Reach_1948	36	188	0.0												18%	-5.4	-5.7	-7.4
di-''isononyl'' phthalate	249-079-5	28553-12-0	28553120	582	Reach_2621	37	419	84.9	3.1E-05	2.7E-03	2.3E+09			2.5E-07	1.1E-07	3.5E-07				24%	-5.6	-5.8	-6.3
naphthalene-2-sulphonic acid	204-375-3	120-18-3	120183	12	Reach_990	38	208	139.2	1.0E-05	2.7E+03	1.0E+00	0.7		1.0E-08	3.5E-08	3.5E-07				23%	-5.0	-5.8	-6.8
2,2'-oxydiethanol	203-872-2	111-46-6	111466	302	Reach_858	39	106	9.0	3.5E-01	4.4E+06	3.4E-02	14.6		2.0E-06	3.5E-07	1.1E-06				14%	-4.8	-5.8	-7.9
potassium formate	209-677-9	590-29-4	590294	1225	Reach_1388	40	84	0.0												18%	-5.5	-5.8	-7.4
1,3,5-trioxane	203-812-5	110-88-3	110883	288	Reach_835	41	90	-54.1	1.4E+03	1.6E+05	2.8E-01			2.2E-09	1.1E-07	3.5E-07				23%	-6.1	-5.8	-6.9
ethylbenzene	202-849-4	100-41-4	100414	124	Reach_556	42	106	-46.9	1.0E+03	1.7E+02	1.1E+03			8.6E-07	3.5E-08	1.1E-07				19%	-6.1	-5.8	-8.3
2,4,6-trichloro-1,3,5-triazine	203-614-9	108-77-0	108770	1489	Reach_755	43	184	68.8	3.1E+00	5.8E+02	5.4E+01		9.8	1.1E-07	3.5E-08	1.1E-07				19%	-5.4	-5.8	-7.4
chloroacetic acid	201-178-4	79-11-8	79118	915	Reach_231	44	94	10.9	3.3E+01	7.0E+05	2.2E+00	2.9		6.9E-07	1.1E-07	3.5E-07				15%	-4.8	-5.8	-7.8
4-nitrotoluene	202-808-0	99-99-0	99990	1095	Reach_545	45	137	38.2	3.7E+00	2.8E+02	2.3E+02			1.3E-08	3.5E-08	1.1E-07				23%	-6.1	-5.8	-7.0
dimethyl terephthalate	204-411-8	120-61-6	120616	1717	Reach_999	46	194	-22.7	3.3E-02	2.0E+03	4.6E+01			1.1E-06	1.1E-07	3.5E-07				14%	-5.6	-5.8	-7.8
4-chloroaniline	203-401-0	106-47-8	106478	193	Reach_669	47	128	24.4	3.2E+00	1.7E+03	5.2E+01		10	5.1E-09	1.1E-07	3.5E-07				23%	-5.4	-5.8	-6.8
diphenylamine	204-539-4	122-39-4	122394	379	Reach_1028	48	169	54.5	1.3E-01	7.3E+01	1.9E+03		13	4.1E-09	1.1E-07	3.5E-07				23%	-5.7	-5.8	-6.8
trisodium nitrilotriacetate	225-768-6	5064-31-3	5064313	1216	Reach_2075	49	257	0.0												18%	-5.5	-5.8	-7.5
ethylenediamine	203-468-6	107-15-3	107153	211	Reach_696	50	60	-23.8	2.4E+03	1.0E+06	2.4E-02		4	4.5E-07	3.5E-07	1.1E-06				15%	-6.1	-5.8	-7.5
sodium benzothiazol-2-yl sulphide	219-660-8	2492-26-4	2492264	1207	Reach_1818	51	189	0.0												18%	-5.5	-5.9	-7.5
dimethylammonium chloride	208-046-5	506-59-2	506592	5899	Reach_1312	52	82	0.0												18%	-5.6	-5.9	-7.5

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
sodium benzoate	208-534-8	532-32-1	532321	1218	Reach_1329	53	144	0.0												18%	-5.6	-5.9	-7.5
4-tert-butylphenol	202-679-0	98-54-4	98544	1073	Reach_511	54	150	36.9	6.0E-01	9.4E+02	2.6E+03	10		2.2E-09	3.5E-07	1.1E-06				23%	-6.1	-5.9	-6.9
2-ethoxy-2-methylpropane	211-309-7	637-92-3	637923	77	Reach_1476	55	102	-81.2	1.7E+04	5.6E+03	8.3E+01			3.3E-09	1.1E-07	3.5E-07				24%	-6.2	-5.9	-8.1
N,N-dimethylformamide	200-679-5	68-12-2	68122	799	Reach_91	56	73	-32.0	4.7E+02	3.4E+06	1.2E-01		14	3.0E-07	1.1E-07	3.5E-07				16%	-6.0	-5.9	-7.7
butane	203-448-7	106-97-8	106978	1451	Reach_686	57	58	-120.3	2.4E+05	5.6E+02	2.0E+02			3.5E-07	1.1E-07	3.5E-07				22%	-6.2	-5.9	-8.8
1-methoxypropan-2-ol	203-539-1	107-98-2	107982	226	Reach_724	58	90	-57.9	9.8E+02	1.0E+06	3.2E-01	15.1		6.4E-07	3.5E-07	1.1E-06				15%	-6.1	-5.9	-7.7
propane	200-827-9	74-98-6	74986	3653	Reach_121	59	44	-133.9	8.2E+05	1.5E+03	6.5E+01			1.1E-06	1.1E-07	3.5E-07				20%	-6.3	-5.9	-8.8
cumene	202-704-5	98-82-8	98828	1076	Reach_518	60	120	-46.3	4.8E+02	8.9E+01	2.8E+03			4.9E-08	3.5E-08	1.1E-07				23%	-6.2	-5.9	-8.2
cyclohexanone	203-631-1	108-94-1	108941	251	Reach_764	61	98	-29.6	5.4E+02	1.5E+04	1.3E+01			8.0E-07	3.5E-07	1.1E-06				15%	-6.2	-5.9	-7.3
(Z)-docos-13-enamide	204-009-2	112-84-5	112845	1607	Reach_926	62	338	183.4	1.1E-05	4.6E-05	2.8E+08	15.1	14.3	1.1E-06	1.1E-07	3.5E-07				23%	-5.8	-5.9	-7.3
bis(2-chloroethoxy)methane	203-920-2	111-91-1	111911	316	Reach_881	63	173	-5.7	1.9E+01	1.7E+04	2.0E+01			1.8E-08	1.1E-07	3.5E-07				22%	-6.2	-5.9	-7.1
2-nitrotoluene	201-853-3	88-72-2	88722	985	Reach_329	64	137	38.2	1.6E+01	5.9E+02	2.3E+02			8.0E-09	3.5E-08	1.1E-07				23%	-6.2	-5.9	-7.2
acrylonitrile	203-466-5	107-13-1	107131	210	Reach_695	65	53	-72.4	1.3E+04	6.9E+04	1.6E+00			5.2E-07	3.5E-07	3.5E-07				16%	-6.2	-6.0	-7.4
tert-butyl hydroperoxide	200-915-7	75-91-2	75912	867	Reach_166	66	90	-41.4	5.1E+03	2.7E+05	8.7E+00	12.7		4.6E-08	3.5E-07	1.1E-06				21%	-6.2	-6.0	-7.1
acrylic acid	201-177-9	79-10-7	79107	914	Reach_230	67	72	-10.4	8.0E+02	1.5E+05	2.8E+00	4.6		4.7E-06	3.5E-07	1.1E-06				14%	-5.4	-6.0	-7.9
cyclohexanol	203-630-6	108-93-0	108930	250	Reach_763	68	100	-33.4	8.7E+01	2.9E+04	4.4E+01	16		8.0E-07	3.5E-07	1.1E-06				15%	-6.2	-6.0	-7.7
methyloxirane	200-879-2	75-56-9	75569	861	Reach_151	69	58	-100.2	7.1E+04	5.8E+04	2.3E+00			6.1E-07	1.1E-07	3.5E-07				17%	-6.3	-6.0	-8.0
morpholine	203-815-1	110-91-8	110918	290	Reach_837	70	87	-15.2	1.5E+03	3.6E+06	2.8E-01		6	3.5E-09	1.1E-07	3.5E-07				23%	-6.3	-6.0	-7.0
Propane-1,2-diol, propoxylated	500-039-8	25322-69-4	25322694	568	Reach_4052	71	308	112.6	9.5E-06	9.5E+02	6.2E-01	14.6		1.8E-07	1.1E-07	3.5E-07				17%	-5.2	-6.0	-7.7
l-(+)-lactic acid	201-196-2	79-33-4	79334	920	Reach_240	72	90	22.7	3.8E+00	7.7E+05	2.2E-01	3.8		4.7E-07	3.5E-07	3.5E-07				15%	-5.0	-6.0	-7.9
p-phenylenediamine	203-404-7	106-50-3	106503	196	Reach_672	73	108	52.8	8.7E-02	2.0E+04	4.1E-01		8	2.2E-09	1.1E-07	1.1E-06				23%	-5.5	-6.0	-7.0
N,N'-ethylenebis[N-acetylacetamide]	234-123-8	10543-57-4	10543574	175	Reach_2295	74	228	186.2	2.0E-06	1.0E+05	4.4E-03		15	4.5E-07	3.5E-07	1.1E-06				15%	-4.9	-6.1	-7.9
sodium chloroacetate	223-498-3	3926-62-3	3926623	1215	Reach_2003	75	116	0.0												18%	-5.8	-6.1	-7.7
p-xylene	203-396-5	106-42-3	106423	189	Reach_665	76	106	-40.7	9.2E+02	1.9E+02	1.2E+03			4.9E-07	3.5E-08	1.1E-07				20%	-6.4	-6.1	-8.4
2-ethylhexanoic acid	205-743-6	149-57-5	149575	479	Reach_1200	77	144	37.7	8.3E+00	5.1E+03	9.1E+02	4.9		6.0E-07	1.1E-07	3.5E-07				15%	-5.9	-6.1	-8.0
bis(4-chlorophenyl) sulphone	201-247-9	80-07-9	80079	3786	Reach_255	78	287	145.5	1.1E-04	3.5E+00	7.9E+03			1.1E-08	3.5E-09	3.5E-09				23%	-6.2	-6.1	-7.1
tetrasodium 4,4'-bis[[4-[bis(2-hydroxyethyl)amino]-6-(4-sulphc	240-521-2	16470-24-9	16470249	5733	Reach_2420	79	1165	0.0												18%	-5.7	-6.1	-7.7
furfuryl alcohol	202-626-1	98-00-0	98000	1063	Reach_494	80	98	-12.4	5.5E+01	1.9E+05	2.8E+00	16		3.1E-07	3.5E-07	1.1E-06				16%	-6.3	-6.1	-7.8
pentasodium (carboxylatomethyl)iminobis(ethylenenitrilo)tetra	205-391-3	140-01-2	140012	1192	Reach_1146	81	503	0.0												18%	-5.8	-6.1	-7.8
pentaerythritol tetrakis(3-(3,5-di-tert-butyl-4-hydroxyphenyl)pı	229-722-6	6683-19-8	6683198	6404	Reach_2202	82	1178	0.0												18%	-5.8	-6.1	-7.8
2-chloroaniline	202-426-4	95-51-2	95512	1031	Reach_431	83	128	24.4	3.1E+01	1.8E+03	5.2E+01		11	2.2E-09	1.1E-07	3.5E-07				23%	-5.7	-6.1	-7.1
butane-1,4-diol	203-786-5	110-63-4	110634	1526	Reach_822	84	90	-8.1	7.3E-01	1.5E+06	6.0E-01	15.5		3.5E-06	3.5E-07	1.1E-06				14%	-5.2	-6.1	-8.2
2-ethylhexan-1-ol	203-234-3	104-76-7	104767	170	Reach_629	85	144	-14.0	5.9E+00	1.4E+02	1.7E+03	15.9		2.9E-07	3.5E-07	1.1E-06				17%	-6.4	-6.1	-7.4
2,4,6-trinitrotoluene	204-289-6	118-96-7	118967	349	Reach_975	86	227	124.4	2.3E-03	2.2E+02	9.8E+01			2.2E-09	3.5E-08	1.1E-07				23%	-6.1	-6.1	-7.1
2-butoxyethanol	203-905-0	111-76-2	111762	309	Reach_869	87	118	-20.3	6.3E+01	7.1E+04	3.7E+00	15		1.0E-06	3.5E-07	1.1E-06				14%	-6.4	-6.1	-8.0
ethylene oxide	200-849-9	75-21-8	75218	854	Reach_134	88	44	-109.3	1.7E+05	2.7E+05	8.9E-01			4.3E-06	1.1E-07	3.5E-07				14%	-6.5	-6.1	-8.0
2,2-dimethylpropane-1,3-diol	204-781-0	126-30-7	126307	1805	Reach_1085	89	104	-1.2	3.3E-01	3.3E+05	1.4E+00	15.3		1.1E-06	3.5E-07	1.1E-06				14%	-5.3	-6.1	-8.1
nitrilotrimethylenetris(phosphonic acid)	229-146-5	6419-19-8	6419198	3429	Reach_2181	90	299	90.3	2.7E-09	1.0E+06	3.5E-06	2.29	3.11	3.5E-07	3.5E-08	1.1E-07				16%	-5.1	-6.2	-8.1
sodium 2-hydroxyethanesulphonate	216-343-6	1562-00-1	1562001	5719	Reach_1692	91	148	0.0												18%	-5.9	-6.2	-7.8
dichloro(dimethyl)silane	200-901-0	75-78-5	75785	3687	Reach_162	92	129	-90.2	1.7E+04	7.1E+03	1.7E+02			3.5E-09	3.5E-09	3.5E-09				24%	-6.6	-6.2	-8.5
2-(2-butoxyethoxy)ethanol	203-961-6	112-34-5	112345	326	Reach_899	93	162	19.3	1.5E+00	5.3E+05	1.9E+00	14.9		7.7E-07	1.1E-07	3.5E-07				15%	-5.5	-6.2	-8.2
di(benzothiazol-2-yl) disulphide	204-424-9	120-78-5	120785	360	Reach_1001	94	332	213.2	8.3E-08	2.0E-03	4.6E+04		11	4.7E-09	1.1E-07	3.5E-07				23%	-6.1	-6.2	-7.1
4-nitrophenol	202-811-7	100-02-7	100027	1	Reach_548	95	139	70.8	3.9E-02	3.8E+04	8.1E+01	7.2		1.1E-08	1.1E-07	3.5E-07				23%	-5.8	-6.2	-7.2
1,5-naphthylenediamine	203-583-1	108-44-1	108441	239	Reach_745	96	107	11.6	4.1E+01	7.3E+03	4.2E+01		9	5.0E-07	1.1E-07	3.5E-07				23%	-5.9	-6.2	-7.1
docusate sodium	209-406-4	577-11-7	577117	1224	Reach_1381	97	445	0.0												18%	-5.9	-6.2	-7.8
pivalic acid	200-922-5	75-98-9	75989	868	Reach_168	98	102	9.9	2.1E+02	6.2E+04	2.8E+01	4.9		2.2E-09	3.5E-07	1.1E-06				23%	-6.3	-6.2	-7.1
1-methyl-2-pyrrolidone	212-828-1	872-50-4	872504	977	Reach_1580	99	99	25.9	4.3E+01	4.4E+06	7.8E-01		14	2.0E-07	3.5E-07	3.5E-06				17%	-6.1	-6.2	-7.9
propan-2-ol	200-661-7	67-63-0	67630	794	Reach_85	100	60	-89.2	6.6E+03	3.6E+05	1.9E+00	16		4.9E-07	1.1E-06	3.5E-06				15%	-6.5	-6.2	-7.5
(1-hydroxyethylidene)bisphosphonic acid, sodium salt	249-559-4	29329-71-3	29329713	5823	Reach_2629	101	229	0.0												18%	-5.9	-6.2	-7.9
benzoic acid	200-618-2	65-85-0	65850	785	Reach_77	102	122	48.9	4.0E-01	3.5E+03	7.4E+01	4.1		1.1E-06	3.5E-07	1.1E-06				14%	-5.6	-6.2	-8.1
edetic acid	200-449-4	60-00-4	60004	71	Reach_53	103	292	315.4	5.0E-10	2.5E+02	1.4E-04	0.67	3.04	5.1E-08	1.1E-07	3.5E-07				21%	-5.3	-6.2	-7.6
o-toluidine	202-429-0	95-53-4	95534	1032	Reach_432	104	107	11.6	4.7E+01	7.6E+03	4.2E+01		10	4.3E-07	1.1E-07	3.5E-07				16%	-5.6	-6.2	-8.1
1-methylpyridinium chloride	662-772-0	25601-41-6	25601416	2440	Reach_4614	105	184	0.4	1.1E+01	3.7E+01	1.5E+04									18%	-5.9	-6.2	-7.9
toluene-4-sulphonic acid	203-180-0	104-15-4	104154	1385	Reach_619	106	172	101.8	3.9E-04	2.8E+03	2.4E-01	0.7		3.5E-07	3.5E-08	1.1E-07				16%	-5.2	-6.2	-8.1
[[(phosphonomethyl)imino]bis[(ethylenenitrilo)bis(methylene)]	244-751-4	22042-96-2	22042962	5777	Reach_2514	107	595	0.0												18%	-5.9	-6.2	-7.9
617-449-9	617-449-9	83196-58-1	83196581	3843	Reach_4463	108	358	190.9	1.2E-08	4.2E+00	1.5E+04	11		3.5E-07	3.5E-08	1.1E-07				17%	-5.6	-6.2	-7.9
buta-1,3-diene	203-450-8	106-99-0	106990	1453	Reach_688	109	54	-123.2	2.7E+05	1.1E+03	1.1E+02			1.1E-06	1.1E-07	3.5E-07				20%	-6.6	-6.2	-9.2
methylammonium nitrate	244-787-0	22113-87-7	22113877	5779	Reach_2517	110	94	0.0												18%	-6.0	-6.2	-7.9
formaldehyde	200-001-8	50-00-0	50000	651	Reach_1	111	30	-110.9	4.7E+05	2.3E+05	2.2E+00			4.6E-06	1.1E-06	3.5E-06				14%	-6.6	-6.2	-7.9
dimethyl phosphonate	212-783-8	868-85-9	868859	976	Reach_1575	112	110	-51.6	2.0E+02	1.9E+05	7.4E-02			2.4E-08	1.1E-07	1.1E-06				22%	-6.5	-6.3	-7.4
resorcinol	203-585-2	108-46-3	108463	240	Reach_747	113	110	45.7	1.6E-02	3.3E+05	1.1E+01	9.6		5.1E-08	3.5E-07	1.1E-06				20%	-5.8	-6.3	-7.6
sodium p-cumenesulphonate	239-854-6	15763-76-5	15763765	5723	Reach_2396	114	222	0.0												18%	-6.0	-6.3	-7.9
tris(2-chloro-1-methylethyl) phosphate	237-158-7	13674-84-5	13674845	24	Reach_2342	115	328	72.3	7.5E-03	3.0E+01	7.8E+02			1.5E-08	3.5E-08	1.1E-07				23%	-6.5	-6.3	-7.4
3-chloro-p-toluidine	214-770-2	1193-21-1	1193211	1689	Reach_1670	116	149	25.6	5.8E+01	2.6E+03	1.7E+01			3.5E-07	3.5E-08	1.1E-07				23%	-6.3	-6.3	-7.3
toluene	203-625-9	108-88-3	108883	247	Reach_760	117	92	-59.2	3.2E+03	4.6E+02	3.5E+02			9.3E-07	3.5E-08	1.1E-07				19%	-6.6	-6.3	-8.8
4,4'-methylenediphenyl diisocyanate	202-966-0	101-68-8	101688	1325	Reach_580	118	250	98.7	2.5E-02	3.5E+01	1.7E+05			1.1E-06	1.1E-07	3.5E-07				18%	-6.4	-6.3	-8.0
[2-(methacryloyloxy)ethyl]trimethylammonium chloride	225-733-5	5039-78-1	5039781	5898	Reach_2073	119	208	0.0												18%	-6.0	-6.3	-7.9
2-nitroaniline	260-480-4	56966-52-0	56966520	3219	Reach_2823	120	289	137.2	2.3E-04	1.4E+00	1.7E+04		11.2	1.1E-06	1.1E-08	3.5E-08				23%	-6.5	-6.3	-7.2
dodecane-12-lactam	213-424-8	947-04-6	947046	4110	Reach_1615	121	197	123.2	4.9E-04	4.8E+01	4.1E+03	15.1	14.3	3.5E-07	3.5E-08	1.1E-07				17%	-6.1	-6.3	-8.0
bis(2-propylheptyl) phthalate	258-469-4	53306-54-0	53306540	3094	Reach_2791	122	447	106.0	4.9E-06	5.7E-04	2.3E+10			1.1E-06	1.1E-07	3.5E-07				24%	-6.3	-6.3	-6.8
dimethyl sulphate	201-058-1	77-78-1	77781	886	Reach_185	123	126	15.1	8.3E+01	1.2E+05	1.4E+00			4.4E-07	1.1E-06	3.5E-06				16%	-6.6	-6.3	-8.0
chloromethane	200-817-4	74-87-3	74873	838	Reach_113	124	50	-124.8	5.4E+05	1.1E+04	1.2E+01			4.3E-08	1.1E-08	3.5E-08				23%	-6.9	-6.3	-8.7
acetone	200-662-2	67-64-1	67641	795	Reach_86	125	58	-93.6	3.3E+04	1.3E+05	5.8E-01			4.7E-06	3.5E-07	1.1E-06				14%	-6.6	-6.3	-8.1
sodium 2-sulphonatoethyl laurate	230-949-8	7381-01-3	7381013	5586	Reach_2244	126	330	0.0												18%	-6.0	-6.3	-8.0
naphthalene	202-049-5	91-20-3	91203	107	Reach_372	127	128	5.0	5.4E+00	9.1E+01	1.5E+03			1.2E-08	3.5E-08	1.1E-07				23%	-6.6	-6.3	-7.6

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
N-(carboxymethyl)-N-(phosphonomethyl)glycine	203-606-5	108-68-9	108689	243	Reach_752	128	122	25.4	3.1E+00	6.7E+03	4.1E+02	10		4.5E-07	1.1E-07	3.5E-07				16%	-5.3	-6.3	-8.3
cyclohexane	203-806-2	110-82-7	110827	285	Reach_830	129	84	-82.7	1.3E+04	1.1E+02	1.5E+03			2.2E-09	1.1E-07	3.5E-07				24%	-6.6	-6.3	-9.1
isononyl alcohol	248-471-3	27458-94-2	27458942	2507	Reach_2605	130	144	-14.0	2.6E+00	1.4E+02	1.7E+03	15.9		1.1E-06	3.5E-07	1.1E-06				15%	-6.6	-6.3	-7.8
formamide	200-842-0	75-12-7	75127	851	Reach_131	131	45	29.0	1.7E+01	1.0E+06	2.5E-02	15.1	14	7.5E-07	1.1E-06	3.5E-06				15%	-5.9	-6.3	-8.3
sodium 2-methyl-2-[(1-oxoallyl)amino]propanesulphonate	225-948-4	5165-97-9	5165979	5908	Reach_2082	132	229	0.0												18%	-6.0	-6.3	-8.0
potassium phenylacetate	201-155-9	78-90-0	78900	904	Reach_215	133	74	-22.9	2.1E+03	1.0E+06	6.3E-02									18%	-6.0	-6.3	-8.0
adiponitrile	203-896-3	111-69-3	111693	307	Reach_865	134	108	21.4	3.4E-01	2.5E+04	2.2E+00			4.4E-07	1.1E-07	3.5E-07				16%	-6.0	-6.3	-8.3
isobutane	200-857-2	75-28-5	75285	3661	Reach_136	135	58	-132.6	3.5E+05	8.6E+02	1.7E+02			1.1E-06	3.5E-07	1.1E-06				20%	-6.7	-6.4	-9.3
2,6-xylenol	209-400-1	576-26-1	576261	723	Reach_1380	136	122	25.4	1.4E+01	3.3E+03	4.1E+02	10.9		3.4E-08	1.1E-07	3.5E-07				21%	-6.6	-6.4	-7.5
2,4-dichlorophenol	202-634-5	98-07-7	98077	1065	Reach_496	137	195	10.4	1.7E+01	2.9E+01	7.9E+03			3.9E-08	3.5E-08	1.1E-07				23%	-6.6	-6.4	-7.3
dimethyl sulfoxide	200-664-3	67-68-5	67685	796	Reach_88	138	78	-55.6	2.6E+02	5.7E+05	1.5E+01			2.2E-09	3.5E-07	3.5E-06				23%	-6.6	-6.4	-7.3
nicotinonitrile	202-863-0	100-54-9	100549	131	Reach_563	139	104	25.4	1.8E+01	1.8E+04	2.2E+00		13	5.5E-09	3.5E-08	1.1E-07				23%	-5.7	-6.4	-7.4
2-(1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol	207-586-9	482-89-3	482893	647	Reach_1292	140	262	190.8	3.1E-09	1.4E+02	1.3E+03		14	3.3E-09	1.1E-07	3.5E-07				23%	-6.0	-6.4	-7.3
methenamine	202-905-8	100-97-0	100970	2	Reach_571	141	140	65.1	1.2E+01	1.0E+06	7.1E-05		9.1	3.7E-07	1.1E-07	3.5E-07				16%	-5.4	-6.4	-8.3
vinyl acetate	203-545-4	108-05-4	108054	228	Reach_727	142	86	-83.5	1.6E+04	2.8E+04	5.4E+00			9.5E-07	3.5E-07	1.1E-06				15%	-6.7	-6.4	-8.2
diallyldimethylammonium chloride	230-993-8	7398-69-8	7398698	1234	Reach_2248	143	162	0.0												18%	-6.1	-6.4	-8.0
triethyl phosphate	201-114-5	78-40-0	78400	894	Reach_198	144	182	3.5	2.2E+01	3.1E+05	7.4E+00			2.6E-08	1.1E-07	3.5E-07				22%	-6.6	-6.4	-7.6
sodium 3,5,6-trichloropyridin-2-olate	202-764-2	99-54-7	99547	1087	Reach_529	145	192	65.7	1.8E+00	7.7E+01	1.3E+03									18%	-6.1	-6.4	-8.1
anthracene	203-697-1	109-70-6	109706	262	Reach_786	146	157	-45.6	7.3E+02	1.7E+03	2.6E+02			8.9E-09	1.1E-08	3.5E-08				23%	-6.6	-6.4	-7.4
2-piperazin-1-ylethylamine	205-411-0	140-31-8	140318	449	Reach_1149	147	129	53.7	8.8E+00	1.0E+06	2.7E-02		4	9.3E-08	1.1E-06	3.5E-06				19%	-6.3	-6.4	-7.9
4,4'-sulphonyldiphenol	201-250-5	80-09-1	80091	97	Reach_257	148	250	176.4	6.3E-08	2.0E+03	4.5E+01	7.7		7.4E-09	1.1E-07	3.5E-07				23%	-5.9	-6.4	-7.4
2-dimethylaminoethanol	203-542-8	108-01-0	108010	227	Reach_725	149	89	-39.6	4.4E+02	1.0E+06	1.1E-01	15	5	6.1E-07	1.1E-06	3.5E-06				15%	-6.7	-6.4	-8.3
ethane	200-814-8	74-84-0	74840	3646	Reach_110	150	30	-147.8	2.7E+06	3.4E+03	2.1E+01			1.1E-06	3.5E-07	1.1E-06				20%	-6.8	-6.4	-9.1
1-chloro-4-nitrobenzene	203-397-0	106-43-4	106434	190	Reach_666	151	127	-27.5	3.0E+02	6.1E+01	1.5E+03			1.3E-08	3.5E-08	1.1E-07				23%	-6.7	-6.4	-7.5
isophthalic acid	204-506-4	121-91-5	121915	1739	Reach_1022	152	166	126.6	3.5E-06	2.8E+03	5.8E+01	3.5		3.5E-06	3.5E-07	1.1E-06				14%	-5.6	-6.4	-8.4
bis(2-ethylhexyl) phthalate	204-211-0	117-81-7	117817	346	Reach_961	153	391	63.9	2.7E-03	1.9E-02	2.5E+08			4.1E-07	1.1E-07	3.5E-07				23%	-6.3	-6.5	-7.7
butan-1-ol	200-751-6	71-36-3	71363	819	Reach_101	154	74	-62.3	1.0E+03	7.5E+04	6.9E+00	15.9		4.0E-06	1.1E-06	3.5E-06				14%	-6.7	-6.5	-8.1
potassium methanolate	212-736-1	865-33-8	865338	6064	Reach_1568	155	70	0.0												18%	-6.2	-6.5	-8.1
troclosene sodium	220-767-7	2893-78-9	2893789	1213	Reach_1880	156	220	0.0												18%	-6.2	-6.5	-8.1
guanidinium nitrate	208-060-1	506-93-4	506934	5900	Reach_1313	157	122	0.0												18%	-6.2	-6.5	-8.1
tris(2-hydroxyethyl)ammonium acetate	238-874-2	14806-72-5	14806725	5702	Reach_2369	158	209	0.0												18%	-6.2	-6.5	-8.1
methane	200-812-7	74-82-8	74828	3645	Reach_108	159	16	-152.9	7.1E+07	2.6E+03	6.0E+00			3.5E-09	3.5E-09	3.5E-09				24%	-7.2	-6.5	-9.1
tris(2,4-ditert-butylphenyl) phosphite	250-709-6	31570-04-4	31570044	2629	Reach_2655	160	647	268.5	6.3E-12	2.2E-11	1.2E+18			1.1E-06	1.1E-07	3.5E-07				24%	-6.7	-6.5	-4.5
2-methoxy-2-methylbutane	213-611-4	994-05-8	994058	4205	Reach_1628	161	102	-81.2	1.0E+04	2.5E+04	8.3E+01			3.5E-07	1.1E-07	3.5E-07				17%	-6.8	-6.5	-8.3
disodium 4,4'-bis[6-anilino-[4-[bis(2-hydroxyethyl)amino]-1,3,5	224-073-5	4193-55-9	4193559	5882	Reach_2020	162	961	0.0												18%	-6.2	-6.5	-8.2
sulphanilic acid	204-482-5	121-57-3	121573	372	Reach_1016	163	173	128.1	3.5E-07	3.9E+04	8.3E-03	0.26	11	5.7E-09	1.1E-07	1.1E-06				23%	-5.8	-6.5	-7.5
2-hydroxybenzimidazole	204-428-0	120-82-1	120821	362	Reach_1003	164	181	16.4	2.4E+01	3.0E+01	8.5E+03			2.4E-09	1.1E-08	3.5E-08				16%	-5.7	-6.5	-8.4
formic acid	200-579-1	64-18-6	64186	777	Reach_71	165	46	-25.0	4.8E+03	2.1E+06	3.5E-01	3.8		4.7E-06	3.5E-07	1.1E-06				14%	-5.3	-6.5	-8.5
methyl methacrylate	201-297-1	80-62-6	80626	938	Reach_268	166	100	-79.6	4.9E+03	3.6E+04	1.9E+01			6.8E-07	3.5E-07	1.1E-06				15%	-6.8	-6.5	-8.0
trichloro(methyl)silane	200-902-6	75-79-6	75796	3689	Reach_163	167	149	-77.1	2.1E+04	3.4E+04	1.0E+02			3.5E-09	3.5E-09	3.5E-09				23%	-6.9	-6.5	-8.6
1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-tria	253-575-7	37640-57-6	37640576	5868	Reach_2711	168	255	0.0												18%	-6.2	-6.5	-8.2
2-pyrrolidone	210-483-1	616-45-5	616455	757	Reach_1432	169	85	46.4	4.7E+00	1.7E+06	4.8E-01	15.1	14	1.8E-07	1.1E-06	3.5E-06				17%	-6.1	-6.5	-8.2
trimethyl-3-[(1-oxoallyl)amino]propylammonium chloride	256-181-3	45021-77-0	45021770	5890	Reach_2757	170	207	0.0												18%	-6.2	-6.5	-8.2
4-chloro-o-cresol	216-381-3	1570-64-5	1570645	495	Reach_1696	171	143	36.2	3.8E+00	1.1E+03	5.0E+02	9.6		3.9E-09	3.5E-07	1.1E-06				23%	-6.8	-6.5	-7.7
thiram (reach)	205-286-2	137-26-8	137268	441	Reach_1137	172	240	107.3	1.5E-03	3.9E+02	5.0E+01		16	2.4E-08	1.1E-07	3.5E-07				22%	-6.0	-6.6	-7.7
3-dimethylaminopropiononitrile	217-090-4	1738-25-6	1738256	2132	Reach_1714	173	98	-23.7	1.8E+02	4.4E+05	3.5E-01		7	1.1E-06	1.1E-07	3.5E-07				14%	-6.7	-6.6	-8.6
2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-N	228-787-8	6358-85-6	6358856	3410	Reach_2171	174	630	349.8	2.9E-19	1.2E-04	1.1E+07	8.45	13.4	3.5E-07	3.5E-08	3.5E-08				16%	-6.3	-6.6	-8.5
2,3,6-trimethylphenol	219-330-3	2416-94-6	2416946	558	Reach_1801	175	136	40.7	2.8E+00	9.5E+02	1.4E+03	10.9		1.6E-08	3.5E-08	1.1E-07				22%	-6.8	-6.6	-7.7
sodium [2-[(2,6-dichlorophenyl)amino]phenyl]acetate	239-346-4	15307-79-6	15307796	30	Reach_2381	176	318	268.5	4.2E-12		3.7E+00	4.35		2.2E-09	1.1E-08	3.5E-08				23%	-5.7	-6.6	-7.5
potassium (R)-(4-hydroxyphenyl)[(3-methoxy-1-methyl-3-oxop	273-992-8	69416-61-1	69416611	6001	Reach_2915	177	303	0.0												18%	-6.3	-6.6	-8.2
butyl acrylate	205-480-7	141-32-2	141322	455	Reach_1161	178	128	-46.0	6.7E+02	1.8E+03	1.6E+02			4.4E-07	3.5E-07	1.1E-06				17%	-6.9	-6.6	-8.3
sodium feredetate	239-802-2	15708-41-5	15708415	1199	Reach_2394	179	367	0.0												18%	-6.3	-6.6	-8.3
2-chloroethanol	203-459-7	107-07-3	107073	207	Reach_692	180	81	-54.0	5.9E+02	2.6E+05	1.3E+00	14.4		4.3E-07	3.5E-08	1.1E-07				16%	-6.9	-6.6	-8.3
phthalonitrile	202-044-8	91-15-6	91156	1004	Reach_369	181	128	58.6	1.1E-01	2.4E+03	1.2E+01			3.7E-08	3.5E-08	1.1E-07				21%	-6.7	-6.6	-7.9
potassium (E,E)-hexa-2,4-dienoate	202-854-1	100-46-9	100469	127	Reach_559	182	107	-0.6	1.0E+02	7.1E+03	1.2E+01									18%	-6.3	-6.6	-8.3
o-phenylenediamine	202-430-6	95-54-5	95545	1033	Reach_433	183	108	52.8	7.1E-03	3.4E+04	1.4E+00		9	3.5E-09	1.1E-07	1.1E-06				23%	-6.1	-6.6	-7.6
3-aminomethyl-3,5,5-trimethylcyclohexylamine	220-666-8	2855-13-2	2855132	2536	Reach_1875	184	170	57.8	4.3E+00	1.4E+05	7.9E+01		3.39	1.1E-06	1.1E-07	3.5E-07				14%	-6.7	-6.6	-8.6
acetic anhydride	203-564-8	108-24-7	108247	234	Reach_737	185	102	-95.1	8.7E+02	2.9E+04	2.6E-01			4.5E-06	3.5E-07	1.1E-06				14%	-6.8	-6.6	-8.3
1-nitroguanidine	209-143-5	556-88-7	556887	707	Reach_1370	186	104	59.9	4.6E-02	1.9E+05	1.9E-02	13	15	4.1E-07	1.1E-07	3.5E-07				16%	-5.5	-6.6	-8.5
3-methylpyridine	203-636-9	108-99-6	108996	253	Reach_767	187	93	-25.9	7.0E+02	5.4E+05	2.2E+01		9	1.2E-08	3.5E-08	1.1E-07				23%	-6.4	-6.6	-7.7
benzyl(methyl)amine	203-133-4	103-67-3	103673	1376	Reach_610	188	121	-9.0	1.3E+02	1.3E+04	3.5E+01		4.3	3.5E-07	3.5E-08	1.1E-07				16%	-6.9	-6.6	-8.0
2-(2-methoxyethoxy)ethanol	203-906-6	111-77-3	111773	310	Reach_870	189	120	-14.6	1.5E+01	1.5E+06	6.6E-02	14.9		8.3E-07	3.5E-07	1.1E-06				15%	-6.2	-6.6	-8.7
pyridine	203-809-9	110-86-1	110861	287	Reach_833	190	79	-44.5	2.6E+03	1.3E+06	6.3E+00		9	7.0E-07	3.5E-08	1.1E-07				15%	-6.1	-6.6	-8.6
anthraquinone	201-549-0	84-65-1	84651	960	Reach_287	191	208	127.6	5.1E-06	1.6E+01	2.2E+03			3.6E-09	1.1E-07	3.5E-07				23%	-6.4	-6.7	-7.6
sodium sarcosinate	224-338-5	4316-73-8	4316738	5885	Reach_2027	192	111	0.0												18%	-6.4	-6.7	-8.3
o-xylene	202-422-2	95-47-6	95476	1028	Reach_428	193	106	-40.7	9.1E+02	1.9E+02	1.2E+03			5.0E-07	3.5E-08	1.1E-07				20%	-7.0	-6.7	-9.0
2,3-epoxypropyltrimethylammonium chloride	221-221-0	3033-77-0	3033770	1214	Reach_1901	194	152	0.0												18%	-6.4	-6.7	-8.3
2-furaldehyde	202-627-7	98-01-1	98011	1064	Reach_495	195	96	-29.5	3.1E+02	6.7E+04	6.8E+00			3.1E-07	3.5E-07	1.1E-06				16%	-6.9	-6.7	-8.1
2-(2-(2-methoxyethoxy)ethoxy)ethanol	203-962-1	112-35-6	112356	1584	Reach_900	196	164	25.0	4.6E-01	3.3E+06	3.5E-02	14.9		1.1E-06	3.5E-07	1.1E-06				14%	-5.7	-6.7	-8.8
2-methylpropene	204-066-3	115-11-7	115117	1631	Reach_937	197	56	-130.9	3.0E+05	1.2E+03	1.7E+02			3.5E-06	3.5E-07	1.1E-06				17%	-7.0	-6.7	-9.9
2,2'-ethylenedioxydiethyl bis(2-ethylhexanoate)	202-319-2	94-28-0	94280	4100	Reach_413	198	403	48.4	5.6E-04	2.0E+00	4.0E+05			3.5E-07	3.5E-08	1.1E-07				20%	-6.7	-6.7	-8.2
N-(1-cyanoethyl)formamide	248-440-4	27394-99-6	27394996	2503	Reach_2604	199	98	70.1	3.9E-01	1.0E+06	6.3E-02	12.2		3.5E-07	3.5E-07	3.5E-07				16%	-5.8	-6.7	-8.6
2,6-xylidine	201-758-7	87-62-7	87627	980	Reach_314	200	121	29.1	2.3E+01	1.7E+03	1.5E+02		10	4.4E-08	3.5E-08	1.1E-07				21%	-6.5	-6.7	-8.0
2,2'-(ethylenedioxy)diethanol	203-953-2	112-27-6	112276	322	Reach_894	201	150	47.2	2.7E-02	9.4E+06	1.8E-02	14.6		1.7E-06	3.5E-07	1.1E-06				14%	-5.6	-6.7	-8.8
tris[2-chloro-1-(chloromethyl)ethyl] phosphate	237-159-2	13674-87-8	13674878	25	Reach_2343	202	431	88.2	3.8E-05	1.9E+00	4.5E+03			1.2E-08	1.1E-08	3.5E-08				23%	-6.8	-6.7	-7.8

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
carbazole	201-696-0	86-74-8	86748	974	Reach_303	203	167	100.2	5.4E-05	8.4E+00	1.7E+03			2.2E-09	3.5E-08	1.1E-07				23%	-6.6	-6.7	-7.6
3,5,5-trimethylcyclohex-2-enone	201-126-0	78-59-1	78591	897	Reach_201	204	138	17.4	3.3E+01	2.0E+03	4.2E+02			2.1E-07	3.5E-07	1.1E-06				17%	-7.0	-6.7	-8.0
cyanamide (reach)	206-992-3	420-04-2	420042	636	Reach_1268	205	42	-36.1	1.9E+03	2.5E+05	1.5E-01		13	7.5E-09	1.1E-07	3.5E-07				23%	-6.0	-6.7	-7.7
(17α)-17-hydroxy-3-oxoandrost-4-ene-17-carbonitrile	278-780-9	77881-13-1	77881131	3742	Reach_2952	206	313	183.0	4.6E-08	5.6E+01	9.1E+02	11		3.5E-07	3.5E-08	1.1E-07				16%	-5.9	-6.7	-8.5
undec-10-enoic acid	203-965-8	112-38-9	112389	1585	Reach_902	207	184	71.5	9.3E-01	3.4E+01	2.3E+04	4.9		3.5E-07	1.1E-07	3.5E-07				16%	-7.0	-6.7	-8.5
methyl acetate	201-185-2	79-20-9	79209	916	Reach_234	208	74	-95.1	7.0E+03	1.7E+05	2.3E+00			9.1E-07	3.5E-07	1.1E-06				15%	-6.9	-6.7	-8.0
1-chloro-2,3-epoxypropane	203-439-8	106-89-8	106898	200	Reach_680	209	93	-65.5	2.4E+03	4.1E+04	4.3E+00			7.7E-07	1.1E-07	3.5E-07				15%	-7.0	-6.7	-8.1
disodium 4,4'-diaminostilbene-2,2'-disulphonate	230-847-3	7336-20-1	7336201	6014	Reach_2239	210	414	0.0												18%	-6.4	-6.7	-8.4
3,3'-dichlorobenzidine dihydrochloride	210-323-0	612-83-9	612839	5949	Reach_1422	211	326	0.0												18%	-6.4	-6.7	-8.4
4-hydroxy-4-methylpentan-2-one	204-626-7	123-42-2	123422	393	Reach_1050	212	116	-10.7	6.5E+01	3.3E+05	4.6E-01	15.2		9.4E-07	3.5E-07	1.1E-06				15%	-6.9	-6.7	-8.7
N-tert-butylbenzothiazole-2-sulphenamide	202-409-1	95-31-8	95318	4124	Reach_425	213	238	127.1	1.1E-03	5.8E+00	3.6E+02		3.4	3.5E-07	3.5E-08	1.1E-07				16%	-7.0	-6.7	-8.5
1-vinyl-2-pyrrolidone	201-800-4	88-12-0	88120	3948	Reach_316	214	111	28.8	1.8E+01	3.7E+05	1.8E+00		14.4	1.1E-06	1.1E-07	3.5E-07				14%	-6.7	-6.7	-8.8
octadecan-1-ol	204-017-6	112-92-5	112925	1611	Reach_930	215	271	86.9	2.4E-04	4.4E-03	5.2E+07	15.9		1.1E-06	3.5E-07	1.1E-06				22%	-6.5	-6.7	-7.9
3-aminophenol	209-711-2	591-27-5	591275	734	Reach_1391	216	109	53.6	2.5E-01	9.3E+04	1.7E+00	9.9	10	3.9E-09	1.1E-07	1.1E-06				23%	-6.3	-6.7	-7.7
p-toluidine	203-403-1	106-49-0	106490	195	Reach_671	217	107	11.6	1.9E-01	7.2E+03	4.2E+01		9	4.3E-07	1.1E-07	3.5E-07				16%	-6.0	-6.7	-8.6
benzothiazole	202-396-2	95-16-9	95169	113	Reach_423	218	135	56.6	9.9E+00	1.1E+03	1.5E+02		11.6	4.8E-09	1.1E-07	3.5E-07				23%	-6.3	-6.7	-7.7
tetrasodium N,N-bis(carboxylatomethyl)-L-glutamate	257-573-7	51981-21-6	51981216	5910	Reach_2777	219	351	0.0												18%	-6.4	-6.7	-8.4
1,3,5-triazine-2,4,6(1H,3H,5H)-trione, trisodium salt	221-255-6	3047-33-4	3047334	5834	Reach_1905	220	195	0.0												18%	-6.4	-6.7	-8.4
butan-2-ol	201-158-5	78-92-2	78922	905	Reach_216	221	74	-76.3	2.7E+03	8.5E+04	5.9E+00	16		4.2E-07	3.5E-07	1.1E-06				16%	-7.0	-6.7	-8.0
sebacic acid	203-845-5	111-20-6	111206	1541	Reach_848	222	202	127.4	8.9E-04	1.1E+03	1.5E+02	4.6		1.1E-06	1.1E-07	3.5E-07				14%	-6.0	-6.7	-8.8
2-hydroxyethyl methacrylate	212-782-2	868-77-9	868779	975	Reach_1574	223	130	-13.0	1.1E+01	5.3E+04	2.0E+00	14.3		6.8E-07	3.5E-07	1.1E-06				15%	-7.0	-6.7	-8.6
[(methylethylene)bis(oxy)]dipropanol	246-466-0	24800-44-0	24800440	2404	Reach_2555	224	192	45.6	6.4E-02	2.2E+04	3.2E-01	14.6		3.5E-07	1.1E-07	3.5E-07				16%	-6.1	-6.8	-8.7
1-aminopropan-2-ol	201-162-7	78-96-6	78966	907	Reach_219	225	75	-28.9	1.0E+02	1.0E+06	6.5E-02	15	5	4.1E-07	1.1E-06	3.5E-06				16%	-6.9	-6.8	-8.6
pyrithione zinc	236-671-3	13463-41-7	13463417	1190	Reach_2336	226	318	0.0												18%	-6.4	-6.8	-8.4
hexamethylene diisocyanate	212-485-8	822-06-0	822060	3822	Reach_1555	227	168	48.8	2.8E+00	3.3E+03	1.6E+03			1.1E-06	3.5E-07	1.1E-06				15%	-7.0	-6.8	-8.6
2-hydroxy-4-(methylthio)butyronitrile	241-756-3	17773-41-0	17773410	2152	Reach_2443	228	131	26.8	2.9E-01	2.7E+04	2.4E-01	10.6		1.1E-06	3.5E-07	1.1E-06				14%	-6.3	-6.8	-8.8
sodium hydroxymethanesulphinate	205-739-4	149-44-0	149440	5704	Reach_1199	229	118	0.0												18%	-6.5	-6.8	-8.4
2-methylglutaronitrile	253-506-0	37439-34-2	37439342	5867	Reach_2710	230	220	0.0												16%	-6.3	-6.8	-8.6
sodium dodecyl sulphate	205-788-1	151-21-3	151213	1198	Reach_1207	231	288	0.0												18%	-6.5	-6.8	-8.4
3,5-dichloroaniline	210-948-9	626-43-7	626437	768	Reach_1457	232	162	46.2	1.1E+00	1.8E+02	2.3E+02		12	2.2E-09	1.1E-08	3.5E-08				23%	-6.0	-6.8	-7.7
pyrazole	224-923-5	4553-62-2	4553622	2942	Reach_2047	233	108	10.7	1.8E+00	2.0E+05	1.9E+00			3.5E-07	1.1E-07	3.5E-07				16%	-5.8	-6.8	-8.7
dichloro(methyl)silane	200-877-1	75-54-7	75547	3675	Reach_149	234	114	-111.6	5.5E+04	4.9E+04	5.0E+01			3.5E-09	3.5E-09	3.5E-09				24%	-7.2	-6.8	-9.0
butanone	201-159-0	78-93-3	78933	906	Reach_217	235	72	-80.5	1.3E+04	2.0E+05	1.8E+00			9.5E-07	3.5E-07	1.1E-06				15%	-7.0	-6.8	-8.1
N-(4-aminophenyl)aniline	202-951-9	101-54-2	101542	1323	Reach_579	236	184	105.5	5.8E-03	1.8E+03	6.6E+01		9.4	1.1E-06	3.5E-07	1.1E-06				14%	-6.1	-6.8	-8.7
sodium hydrogen glutamate	205-538-1	142-47-2	142472	5695	Reach_1178	237	169	0.0												18%	-6.5	-6.8	-8.4
benzyl alcohol	202-859-9	100-51-6	100516	129	Reach_561	238	108	-5.4	7.1E+00	2.4E+04	1.2E+01	14.9		1.1E-06	3.5E-07	1.1E-06				14%	-7.0	-6.8	-8.7
butyraldehyde	204-646-6	123-72-8	123728	396	Reach_1056	239	72	-80.2	1.4E+04	5.0E+04	6.6E+00			4.1E-06	1.1E-06	3.5E-06				14%	-7.1	-6.8	-8.6
2-chloropyridine	203-646-3	109-09-1	109091	255	Reach_770	240	114	-12.6	2.1E+02	1.0E+03	2.8E+01		13	2.2E-09	3.5E-08	1.1E-07				23%	-6.0	-6.8	-7.7
dimethylammonium 2,4-dichlorophenoxyacetate	217-915-8	2008-39-1	2008391	1202	Reach_1744	241	266	0.0												18%	-6.5	-6.8	-8.4
C,C'-azodi(formamide)	204-650-8	123-77-3	123773	1775	Reach_1058	242	116	117.0	1.4E-03	1.5E+05	1.3E-04	14	14	1.1E-06	3.5E-07	1.1E-06				14%	-5.8	-6.8	-8.9
tetrasodium (1-hydroxyethylidene)bisphosphonate	223-267-7	3794-83-0	3794830	5869	Reach_1992	243	294	0.0												18%	-6.5	-6.8	-8.5
tetrahydrothiophene 1,1-dioxide	204-783-1	126-33-0	126330	406	Reach_1086	244	120	16.3	5.5E-01	3.4E+04	5.8E-01			2.2E-09	1.1E-07	3.5E-07				23%	-6.7	-6.8	-7.7
2,4,6-tribromophenol	204-278-6	118-79-6	118796	348	Reach_970	245	331	107.2	4.0E-02	1.6E+01	1.5E+04	6.2		2.3E-08	1.1E-07	3.5E-07				22%	-7.1	-6.8	-7.9
1,4-diazabicyclooctane	205-999-9	280-57-9	280579	577	Reach_1219	246	112	20.6	6.6E+00	1.0E+06	3.2E-01		5	3.7E-09	3.5E-07	3.5E-06				23%	-6.8	-6.8	-7.8
3,5-xylenol	204-680-1	124-10-7	124107	1784	Reach_1068	247	242	35.9	3.4E-01	6.0E-01	1.9E+06			1.1E-06	1.1E-07	3.5E-07				16%	-7.1	-6.8	-8.6
dodecan-1-ol	203-982-0	112-53-8	112538	332	Reach_911	248	186	29.2	2.4E-01	5.8E+00	5.9E+04	15.9		3.6E-06	1.1E-07	3.5E-07				16%	-7.1	-6.8	-8.5
2,5-dichloroaniline	202-455-2	95-82-9	95829	1040	Reach_444	249	162	46.2	2.0E+00	1.8E+02	2.3E+02		12	2.3E-09	1.1E-08	3.5E-08				23%	-6.0	-6.8	-7.8
ethyl acetate	205-500-4	141-78-6	141786	458	Reach_1168	250	88	-82.1	1.3E+04	3.8E+04	7.2E+00			9.1E-07	3.5E-07	1.1E-06				15%	-7.1	-6.8	-8.5
dimethylamine	204-697-4	124-40-3	124403	17	Reach_1077	251	45	-106.2	2.0E+05	1.0E+06	6.8E-01		3.3	5.1E-07	1.1E-07	3.5E-07				16%	-7.2	-6.8	-8.1
2-methylbutane	201-142-8	78-78-4	78784	3758	Reach_208	252	72	-119.0	9.2E+04	3.0E+02	5.2E+02			1.1E-06	3.5E-07	1.1E-06				20%	-7.1	-6.8	-9.9
cyanoguanidine	207-312-8	461-58-5	461585	2948	Reach_1283	253	84	44.8	5.1E+00	2.6E+05	4.6E-02	13	14.9	1.1E-06	3.5E-07	1.1E-06				14%	-5.7	-6.8	-8.8
p-cresol	203-398-6	106-44-5	106445	191	Reach_667	254	108	15.7	1.7E+01	1.6E+04	1.1E+02	10		7.1E-07	1.1E-06	3.5E-06				15%	-7.1	-6.8	-8.6
1,1',1''-nitrilotripropan-2-ol	204-528-4	122-20-3	122203	1743	Reach_1027	255	191	78.6	2.5E-03	2.6E+06	6.0E-02	14.5	6.2	1.1E-06	3.5E-07	1.1E-06				14%	-5.8	-6.8	-8.9
[3-methyl-5-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4-pentadieny	212-028-2	751-83-7	751837	6024	Reach_1525	256	1027	0.0												18%	-6.5	-6.8	-8.5
(4-chlorophenyl)hydrazine	202-446-3	95-74-9	95749	1037	Reach_439	257	142	41.8	5.0E+00	5.6E+02	1.9E+02		10	6.9E-09	3.5E-07	1.1E-06				16%	-6.2	-6.8	-8.7
2-hydroxyethyl acrylate	212-454-9	818-61-1	818611	943	Reach_1552	258	116	-15.9	1.7E+01	2.3E+05	5.6E-01	14.3		4.4E-07	3.5E-07	1.1E-06				16%	-7.0	-6.8	-8.7
2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-d	225-822-9	5102-83-0	5102830	3025	Reach_2078	259	686	349.8	6.2E-21	1.5E-06	1.3E+08	8.45	13.4	3.5E-07	3.5E-08	3.5E-08				16%	-6.5	-6.8	-8.7
tris(2-ethylhexyl) benzene-1,2,4-tricarboxylate	222-020-0	3319-31-1	3319311	2676	Reach_1945	260	547	197.0	7.8E-06	3.2E-05	3.9E+11			1.1E-06	1.1E-07	3.5E-07				24%	-7.0	-6.8	-7.4
p-cumenesulphonic acid	240-210-1	16066-35-6	16066356	2076	Reach_2410	261	200	110.8	1.1E-04	2.5E+03	1.9E+00	0.7		3.5E-07	3.5E-08	1.1E-07				16%	-5.8	-6.8	-8.8
sodium hydrogen 4-amino-5-hydroxynaphthalene-2,7-disulpho	226-736-4	5460-09-3	5460093	5583	Reach_2116	262	341	0.0												18%	-6.5	-6.8	-8.5
tetradecanol	204-000-3	112-72-1	112721	1599	Reach_920	263	214	49.4	2.7E-02	5.2E-01	5.6E+05	15.9		1.1E-06	3.5E-07	1.1E-06				19%	-7.0	-6.9	-8.3
4-methyl-m-phenylenediamine	202-453-1	95-80-7	95807	1039	Reach_443	264	122	67.3	7.6E-02	3.5E+04	1.4E+00		9	2.2E-09	1.1E-07	3.5E-07				23%	-6.2	-6.9	-7.8
2-methylpentane-2,4-diol	203-489-0	107-41-5	107415	219	Reach_706	265	118	-7.4	7.8E+00	5.3E+05	3.8E+00	15.4		4.1E-07	3.5E-07	1.1E-06				16%	-6.7	-6.9	-8.7
4-tert-butylbenzoic acid	202-696-3	98-73-7	98737	1075	Reach_517	266	178	80.9	1.1E-02	2.6E+00	6.0E+03	4.1		1.5E-08	3.5E-07	1.1E-06				22%	-6.8	-6.9	-8.0
2-(2-ethoxyethoxy)ethanol	203-919-7	111-90-0	111900	315	Reach_880	267	134	-3.1	1.3E+01	1.8E+06	2.0E-01	14.9		8.1E-07	1.1E-07	3.5E-07				15%	-6.4	-6.9	-9.0
4-chlorophenol	203-402-6	106-48-9	106489	194	Reach_670	268	129	28.6	5.3E+00	1.1E+04	1.4E+02	9.6		2.2E-09	1.1E-07	3.5E-07				23%	-7.1	-6.9	-7.8
4-(1,1,3,3-tetramethylbutyl)phenol	205-426-2	140-66-9	140669	451	Reach_1150	269	206	72.8	6.9E-02	1.6E+01	1.9E+05	10		4.5E-09	3.5E-07	1.1E-06				23%	-6.9	-6.9	-8.0
L-menthol	218-690-9	2216-51-5	2216515	538	Reach_1773	270	156	-5.9	1.0E+00	9.4E+02	2.4E+03	16		3.2E-07	1.1E-07	3.5E-07				17%	-7.1	-6.9	-8.5
diclofenac	239-348-5	15307-86-5	15307865	31	Reach_2382	271	296	174.6	8.2E-06	1.6E+01	1.0E+04	4.35		2.2E-09	1.1E-07	1.1E-07				23%	-6.7	-6.9	-7.8
disodium dihydrogen ethylenediaminetetraacetate	205-358-3	139-33-3	139333	5686	Reach_1143	272	336	0.0												18%	-6.6	-6.9	-8.5
N,N''-(isobutylidene)diurea	228-055-8	6104-30-9	6104309	3324	Reach_2153	273	174	141.0	7.8E-04	2.3E+01	2.1E-02	13.5	14	1.1E-06	3.5E-07	1.1E-06				14%	-6.7	-6.9	-9.0
1,3-dimethylurea	202-498-7	96-31-1	96311	1052	Reach_460	274	88	20.2	2.0E-01	1.7E+05	2.4E-01	14.3	14	7.2E-09	1.1E-07	3.5E-07				23%	-6.3	-6.9	-7.9
[[(phosphonomethyl)imino]bis[ethane-2,1-diylnitrilobis(methyl	239-931-4	15827-60-8	15827608	2059	Reach_2401	275	573	90.3	2.7E-09	1.0E+06	1.9E-10	0.37	2.61	3.5E-07	1.1E-07	3.5E-07				16%	-5.8	-6.9	-8.8
m-phenylenebis(methylamine)	216-032-5	1477-55-0	1477550	1997	Reach_1686	276	136	60.1	1.9E+00	2.6E+03	1.4E+00		4.59	3.5E-07	3.5E-08	1.1E-07				16%	-7.2	-6.9	-8.7
O-benzyl-L-valine toluene-p-sulphonate	240-702-6	16652-76-9	16652769	5735	Reach_2425	277	379	0.0												18%	-6.6	-6.9	-8.5

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
N-methylaniline	253-657-2	37763-23-8	37763238	2807	Reach_2712	278	181	88.3	2.0E-02	3.1E+04	1.1E+00		12.5	1.1E-05	1.1E-06	3.5E-06				23%	-7.1	-6.9	-7.8
disodium 4,4'-bis[(4-anilino-6-morpholino-1,3,5-triazin-2-yl)am	240-245-2	16090-02-1	16090021	1200	Reach_2412	279	925	0.0												18%	-6.6	-6.9	-8.6
tris(nonylphenyl) phosphite	247-759-6	26523-78-4	26523784	2474	Reach_2585	280	689	317.3	2.6E-15	2.8E-13	1.1E+20			1.1E-06	1.1E-07	3.5E-07				24%	-7.1	-6.9	-3.9
o-cresol	202-423-8	95-48-7	95487	1029	Reach_429	281	108	15.7	3.3E+01	1.7E+04	1.1E+02	10		6.7E-07	1.1E-06	3.5E-06				15%	-7.1	-6.9	-8.6
potassium hydrogen oxalate	204-873-0	127-95-7	127957	5652	Reach_1103	282	128	0.0												18%	-6.6	-6.9	-8.5
bis(pentane-2,4-dionato)calcium	243-001-3	19372-44-2	19372442	5757	Reach_2477	283	238	0.0												18%	-6.6	-6.9	-8.5
2,4,5-trichloroaniline	211-254-9	636-30-6	636306	774	Reach_1474	284	196	71.0	2.6E-01	2.7E+01	1.0E+03		13	2.2E-09	1.1E-08	3.5E-08				23%	-6.4	-6.9	-7.8
1,1'-iminodipropan-2-ol	203-820-9	110-97-4	110974	292	Reach_840	285	133	25.8	1.7E-01	1.0E+06	1.3E-01	14.7	5	3.4E-07	1.1E-06	3.5E-06				16%	-6.2	-6.9	-8.7
potassium 2-ethylhexanoate	221-625-7	3164-85-0	3164850	5842	Reach_1924	286	182	0.0												18%	-6.6	-6.9	-8.5
2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-chl	226-939-8	5567-15-7	5567157	706	Reach_2124	287	819	349.8	2.4E-23	1.9E-06	3.5E+07	8.45	15	1.2E-07	3.5E-09	1.1E-08				19%	-6.7	-6.9	-8.5
bis(pentabromophenyl) ether	214-604-9	1163-19-5	1163195	345	Reach_1664	288	959	254.5	6.2E-10	1.9E-10	1.3E+12			2.5E-09	1.1E-07	3.5E-07							
6-aminopenicillanic acid	208-993-4	551-16-6	551166	3161	Reach_1357	289	216	296.2	2.4E-07	5.8E+03	4.0E+00	4	7.04	3.5E-07	1.1E-07	3.5E-07				16%	-5.9	-6.9	-8.8
2-(2-pyridyl)ethanol	203-140-2	103-74-2	103742	163	Reach_614	290	123	38.5	1.2E+00	7.0E+03	2.4E+00	15	9	2.7E-08	1.1E-07	3.5E-07				22%	-6.3	-6.9	-8.1
dichloromethane	200-838-9	75-09-2	75092	850	Reach_129	291	85	-89.5	5.8E+04	1.8E+04	2.2E+01			2.0E-08	1.1E-08	3.5E-08				23%	-7.3	-6.9	-9.2
17β-hydroxy-17-(3-hydroxy-1-propynyl)androst-4-ene-3-one	259-700-1	55542-26-2	55542262	3172	Reach_2807	292	342	196.3	1.6E-09	4.6E-01	8.5E+02	13.2		1.1E-06	1.1E-07	3.5E-07				15%	-6.1	-6.9	-8.8
pentane	203-692-4	109-66-0	109660	260	Reach_783	293	72	-106.9	6.8E+04	3.2E+02	6.3E+02			1.6E-06	1.1E-07	3.5E-07				19%	-7.2	-6.9	-10.0
3-chloropropane-1,2-diol	202-492-4	96-24-2	96242	1050	Reach_457	294	111	-1.9	3.5E+00	1.1E+06	3.0E-01	13.7		6.9E-07	3.5E-07	1.1E-06				15%	-6.3	-6.9	-8.9
1-naphthylamine	700-846-7	274693-53-7	274693537	2508	Reach_5010	295	307	154.8	6.2E-07	1.1E+03	1.6E+02			1.1E-06	3.5E-07	1.1E-06				23%	-6.6	-6.9	-8.0
1-chloro-2-nitrobenzene	201-854-9	88-73-3	88733	986	Reach_330	296	158	48.8	3.8E+00	3.8E+02	2.9E+02			2.2E-09	1.1E-07	3.5E-07				23%	-7.2	-6.9	-8.1
tetrakis(hydroxymethyl)phosphonium chloride	204-707-7	124-64-1	124641	5637	Reach_1080	297	191	0.0												18%	-6.6	-6.9	-8.6
methacrylic acid	201-204-4	79-41-4	79414	3776	Reach_245	298	86	-7.0	2.9E+02	9.7E+04	9.8E+00	4.6		3.5E-06	3.5E-07	1.1E-06				14%	-6.4	-6.9	-8.9
11-aminoundecanoic acid	219-417-6	2432-99-7	2432997	2387	Reach_1808	299	201	304.1	2.1E-07	1.6E+01	6.9E-01	4.89	3.49	1.1E-06	1.1E-07	3.5E-07				14%	-5.8	-6.9	-9.0
methoxyammonium chloride	604-045-2	137862-53-4	137862534	442	PharmaBeta_775	300	436	294.1	1.1E-13	1.3E-02	4.5E+03									18%	-6.6	-6.9	-8.6
3,5,7-triaza-1-azoniatricyclo[3.3.1.13,7]decane nitrate	687-538-5	18423-20-6	18423206	5747	Reach_4635	301	203	0.0												18%	-6.6	-6.9	-8.6
tris(2-butoxyethyl) phosphate	201-122-9	78-51-3	78513	93	Reach_200	302	398	85.8	1.6E-04	2.4E+00	1.0E+03			3.0E-08	1.1E-07	3.5E-07				22%	-7.2	-6.9	-8.2
tributyl phosphate	204-800-2	126-73-8	126738	19	Reach_1089	303	266	64.7	4.7E-01	1.0E+03	6.6E+03			2.6E-08	1.1E-07	3.5E-07				22%	-7.1	-6.9	-8.1
propylenediamine	235-845-6	13005-36-2	13005362	5655	Reach_2316	304	174	0.0												17%	-7.2	-6.9	-8.4
1,2-dichloro-3-nitrobenzene	221-717-7	3209-22-1	3209221	600	Reach_1932	305	192	65.7	1.1E+00	7.9E+01	1.3E+03			2.3E-09	1.1E-08	3.5E-08				23%	-7.2	-6.9	-8.2
phthalimide	201-603-3	85-41-6	85416	965	Reach_294	306	147	177.3	1.4E-06	3.4E+03	2.0E+01	9.3		3.5E-07	3.5E-07	1.1E-06				16%	-6.2	-6.9	-8.7
tripotassium citrate	212-755-5	866-84-2	866842	6068	Reach_1571	307	306	0.0												18%	-6.6	-6.9	-8.6
2,2,6,6-tetramethylpiperidin-4-ol	219-291-2	2403-88-5	2403885	2368	Reach_1797	308	157	52.7	4.2E-01	2.3E+03	8.7E+00	15.1	4.4	1.1E-06	3.5E-07	1.1E-06				14%	-7.2	-7.0	-8.9
dinoseb	201-861-7	88-85-7	88857	989	Reach_333	309	240	138.0	9.9E-03	2.7E+02	4.7E+03	4.2		8.3E-09	3.5E-08	1.1E-07				23%	-6.8	-7.0	-8.0
benzophenone	204-337-6	119-61-9	119619	354	Reach_982	310	182	63.6	1.2E-01	4.8E+01	1.4E+03			2.5E-09	1.1E-07	3.5E-07				23%	-7.2	-7.0	-8.1
disodium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4-)-M	239-407-5	15375-84-5	15375845	5714	Reach_2386	311	389	0.0												18%	-6.6	-7.0	-8.6
tetrasodium 4-amino-5-hydroxy-3,6-bis[[4-[[2-(sulphonatooxy)	241-164-5	17095-24-8	17095248	5738	Reach_2430	312	992	0.0												18%	-6.6	-7.0	-8.6
atrazine (reach)	217-617-8	1912-24-9	1912249	37	Reach_1734	313	216	113.9	3.8E-03	1.5E+01	6.6E+02		12.3	2.2E-09	1.1E-07	1.1E-07				23%	-6.7	-7.0	-7.9
phenylhydrazine	202-873-5	100-63-0	100630	134	Reach_565	314	108	25.2	5.1E+00	3.7E+05	6.2E+00		5	4.6E-08	1.1E-07	3.5E-07				21%	-6.9	-7.0	-8.3
chloroform	200-663-8	67-66-3	67663	83	Reach_87	315	119	-78.9	2.5E+04	6.6E+03	3.3E+01			2.9E-08	1.1E-08	3.5E-08				23%	-7.4	-7.0	-9.4
dimethyl phthalate	205-011-6	131-11-3	131113	417	Reach_1119	316	194	-22.7	6.2E-01	2.0E+03	4.6E+01			7.9E-07	1.1E-07	3.5E-07				15%	-7.2	-7.0	-8.9
propionic acid	201-176-3	79-09-4	79094	913	Reach_229	317	74	-9.0	8.1E+02	3.5E+05	3.8E+00	4.9		4.7E-06	3.5E-07	1.1E-06				14%	-6.4	-7.0	-8.9
benzothiazole-2-thiol	205-736-8	149-30-4	149304	478	Reach_1198	318	167	85.8	5.6E-03	1.4E+02	7.2E+02	6.9		5.4E-09	1.1E-07	3.5E-07				23%	-7.1	-7.0	-8.0
ibuprofen	258-868-3	53928-30-6	53928306	3115	Reach_2795	319	491	240.3	5.3E-10	1.7E-01	3.7E+05			3.5E-07	3.5E-08	1.1E-07				22%	-6.8	-7.0	-8.1
ethylene dinitrate	211-063-0	628-96-6	628966	3382	Reach_1462	320	152	-10.1	5.2E+01	5.4E+04	1.5E+01			1.1E-06	3.5E-08	1.1E-07				14%	-7.2	-7.0	-8.9
anilinoacetonitrile	221-129-0	3009-97-0	3009970	2585	Reach_1897	321	132	45.3	1.2E+00	6.5E+04	1.4E+01		14.6	3.5E-07	1.1E-07	3.5E-07				16%	-6.2	-7.0	-8.8
2-phenoxyethanol	204-589-7	122-99-6	122996	384	Reach_1036	322	138	22.5	6.0E-01	6.3E+03	1.3E+01	14.8		6.9E-07	3.5E-07	1.1E-06				15%	-7.2	-7.0	-8.9
disodium [[N,N'-ethylenediylbis[N-(carboxylatomethyl)glycinat	237-865-0	14025-21-9	14025219	1194	Reach_2355	323	400	0.0												18%	-6.7	-7.0	-8.6
4,4'-methylenedianiline	202-974-4	101-77-9	101779	1328	Reach_582	324	198	127.5	2.8E-04	4.9E+02	1.5E+02		8.72	1.1E-06	1.1E-07	3.5E-07				14%	-6.3	-7.0	-9.0
sodium dibutyldithiocarbamate	205-238-0	136-30-1	136301	5676	Reach_1135	325	227	0.0												18%	-6.7	-7.0	-8.6
m-toluidine	601-639-3	119851-28-4	119851284	1700	Reach_4098	326	281	124.2	7.5E-04	4.0E+00	1.0E+05			1.1E-06	3.5E-08	1.1E-07				15%	-7.0	-7.0	-8.9
2,2',2''-(hexahydro-1,3,5-triazine-1,3,5-triyl)triethanol	225-208-0	4719-04-4	4719044	117	Reach_2059	327	219	155.3	5.5E-07	1.0E+06	2.1E-05	14.1	11	7.1E-07	1.1E-06	3.5E-06				15%	-5.9	-7.0	-8.9
potassium sodium tartrate	206-156-8	304-59-6	304596	5833	Reach_1230	328	210	0.0												18%	-6.7	-7.0	-8.7
sodium N-lauroylsarcosinate	205-281-5	137-16-6	137166	5680	Reach_1136	329	293	0.0												18%	-6.7	-7.0	-8.7
17β-hydroxy-17-(3-hydroxypropyl)androst-4-ene-4-one	259-701-7	55542-27-3	55542273	3173	Reach_2808	330	347	192.4	3.2E-09	3.5E+01	4.5E+03	15.5		1.1E-06	1.1E-07	3.5E-07				15%	-6.2	-7.0	-8.8
sodium ethylenesulphonate	221-242-5	3039-83-6	3039836	5832	Reach_1903	331	130	0.0												18%	-6.7	-7.0	-8.7
3a,4,7,7a-tetrahydro-4,7-methanoindene	201-052-9	77-73-6	77736	884	Reach_182	332	132	-16.8	2.2E+02	9.1E+02	1.4E+03			9.0E-08	1.1E-07	3.5E-07				20%	-7.3	-7.0	-8.6
tetrasodium 4,4'-bis[[4-[bis(2-hydroxypropyl)amino]-6-[(4-sulp	267-097-1	67786-25-8	67786258	5986	Reach_2887	333	1221	0.0												18%	-6.7	-7.0	-8.7
1-(aminomethyl)cyclohexaneacetic acid hydrochloride	262-075-8	60142-95-2	60142952	5945	Reach_2845	334	208	0.0												18%	-6.7	-7.0	-8.7
N-Pentanoyl-N-{[2'-(1H-tetrazol-5-yl)biphenyl-4-yl]methyl}-L-va	618-706-8	91161-71-6	91161716	4012	Reach_4498	335	291	146.5	7.8E-05	2.0E+00	6.5E+05			1.1E-06	3.5E-08	1.1E-07				18%	-6.6	-7.0	-8.7
disodium [2,2'-bi-1H-indole]-3,3'-diolate	212-974-6	894-86-0	894860	6077	Reach_1586	336	308	0.0												18%	-6.7	-7.0	-8.7
aminoiminomethanesulphinic acid	217-157-8	1758-73-2	1758732	2144	Reach_1717	337	108	0.0						3.5E-06	3.5E-07	1.1E-06				18%	-6.7	-7.0	-8.7
2-phenylpropene	202-705-0	98-83-9	98839	4193	Reach_519	338	118	-45.0	2.6E+02	2.7E+02	2.8E+03			3.5E-07	3.5E-08	1.1E-07				19%	-7.3	-7.0	-9.0
4-chloro-2-nitroaniline	201-925-4	89-63-4	89634	992	Reach_348	339	173	93.2	3.7E-02	4.1E+02	4.6E+02		15	2.2E-09	1.1E-07	3.5E-07				23%	-6.8	-7.0	-8.0
benzotriazole	202-394-1	95-14-7	95147	112	Reach_422	340	119	85.2	3.3E-03	7.7E+03	1.5E+01	8.5	12.4	5.7E-09	1.1E-07	3.5E-07				23%	-6.5	-7.0	-8.0
1-butoxypropan-2-ol	225-878-4	5131-66-8	5131668	3032	Reach_2080	341	132	-21.7	5.3E+01	1.5E+04	9.5E+00	15.1		3.5E-07	1.1E-07	3.5E-07				16%	-7.3	-7.0	-8.6
sodium hydrogen 2-aminobenzene-1,4-disulphonate	214-222-2	1115-20-4	1115204	1550	Reach_1648	342	204	80.9	2.2E-03	4.6E+03	1.2E+01									18%	-6.7	-7.0	-8.7
triphenylphosphine	210-036-0	603-35-0	603350	751	Reach_1412	343	262	108.7	1.4E-03	4.9E+00	1.0E+05			2.6E-08	3.5E-09	1.1E-08				23%	-7.3	-7.0	-8.2
sodium 2,4-dichlorophenoxyacetate	220-290-4	2702-72-9	2702729	1210	Reach_1856	344	243	0.0												18%	-6.7	-7.0	-8.7
2-dimethylaminoethyl methacrylate	220-688-8	2867-47-2	2867472	583	Reach_1878	345	157	-20.5	9.6E+01	8.3E+04	9.3E+00		6	5.5E-07	3.5E-07	1.1E-06				15%	-7.3	-7.0	-8.8
1-ethoxypropan-2-ol	216-374-5	1569-02-4	1569024	2053	Reach_1694	346	104	-45.6	5.1E+02	2.3E+05	1.0E+00	15.1		1.1E-06	3.5E-07	1.1E-06				14%	-7.3	-7.0	-8.8
3-(methylthio)propionaldehyde	221-882-5	3268-49-3	3268493	2658	Reach_1939	347	104	-43.5	2.6E+02	2.3E+04	2.6E+00			3.5E-06	1.1E-06	3.5E-06				14%	-7.3	-7.1	-8.7
n-butyl acetate	204-658-1	123-86-4	123864	397	Reach_1059	348	116	-56.8	1.6E+03	4.0E+03	7.1E+01			9.2E-07	3.5E-07	1.1E-06				16%	-7.3	-7.1	-8.8
but-1-ene	203-449-2	106-98-9	106989	1452	Reach_687	349	56	-121.7	2.5E+05	1.1E+03	1.5E+02			1.1E-06	1.1E-07	3.5E-07				20%	-7.4	-7.1	-10.0
titanium tetrabutanolate	227-006-8	5593-70-4	5593704	5934	Reach_2129	350	388	0.0												18%	-6.7	-7.1	-8.7
4,4'-diaminostilbene-2,2'-disulphonic acid	201-325-2	81-11-8	81118	3801	Reach_271	351	370	283.1	1.4E-16	6.4E-01	3.8E-02	-1.15	9.97	3.5E-06	1.1E-07	3.5E-07				14%	-5.8	-7.1	-9.3
1-methylpiperazine	203-639-5	109-01-3	109013	254	Reach_768	352	100	19.0	9.3E+02	1.0E+06	2.6E-01		5	2.2E-09	1.1E-06	3.5E-06				23%	-7.3	-7.1	-8.1

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
2-(2-aminoethylamino)ethanol	203-867-5	111-41-1	111411	1547	Reach_855	353	104	25.8	8.8E-01	1.0E+06	7.4E-03	14.9	4.35	3.5E-06	1.1E-06	3.5E-06				14%	-6.2	-7.1	-9.1
palmitic acid	200-312-9	57-10-3	57103	3222	Reach_37	354	256	116.4	7.4E-03	4.3E-01	9.1E+06	4.9		1.1E-06	1.1E-07	3.5E-07				16%	-7.2	-7.1	-9.0
hexadecan-1-ol	253-149-0	36653-82-4	36653824	615	Reach_2702	355	242	68.6	1.2E-03	2.1E-02	5.4E+06	15.9		3.5E-06	3.5E-07	1.1E-06				20%	-7.2	-7.1	-8.7
1,1'-(ethane-1,2-diyl)bis[pentabromobenzene]	284-366-9	84852-53-9	84852539	3878	Reach_2982	356	971	259.7	2.5E-11	2.6E-11	4.4E+13			3.5E-07	3.5E-08	1.1E-07				24%	-7.3	-7.1	-7.0
succinic acid	203-740-4	110-15-6	110156	274	Reach_805	357	118	83.3	1.4E-02	3.8E+05	1.8E-01	3.8		9.4E-07	3.5E-07	1.1E-06				15%	-6.0	-7.1	-9.0
sodium etasulfate	204-812-8	126-92-1	126921	5646	Reach_1091	358	232	0.0												18%	-6.8	-7.1	-8.7
methyl formate	203-481-7	107-31-3	107313	1459	Reach_704	359	60	-99.5	7.9E+04	2.0E+05	6.8E-01			3.5E-06	3.5E-07	1.1E-06				14%	-7.4	-7.1	-9.0
menthol	201-939-0	89-78-1	89781	994	Reach_351	360	156	-5.9	1.0E+00	9.4E+02	2.4E+03	16		3.2E-07	1.1E-07	3.5E-07				17%	-7.3	-7.1	-8.7
o-anisidine	201-963-1	90-04-0	90040	999	Reach_357	361	123	28.6	1.4E+01	1.1E+04	1.4E+01		9	6.0E-07	1.1E-07	1.1E-06				15%	-6.8	-7.1	-9.0
2-(2-aminoethoxy)ethanol	213-195-4	929-06-6	929066	4053	Reach_1603	362	105	13.9	3.3E+00	1.0E+06	1.3E-02	14.9	4.56	1.1E-06	3.5E-07	1.1E-06				14%	-6.4	-7.1	-9.2
N-cyclohexylbenzothiazole-2-sulfenamide	202-411-2	95-33-0	95330	4125	Reach_426	363	264	151.3	2.4E-04	1.7E+00	3.0E+03		3.4	1.1E-06	1.1E-07	3.5E-07				15%	-7.3	-7.1	-9.0
tetrahydrofuran	203-726-8	109-99-9	109999	269	Reach_798	364	72	-84.9	2.3E+04	5.1E+04	8.7E+00			1.1E-06	1.1E-07	3.5E-07				15%	-7.4	-7.1	-8.9
(2R,5R)-1,6-Diphenylhexane-2,5-diamine dihydrochloride	203-052-4	102-77-2	102772	1353	Reach_598	365	252	150.7	6.8E-04	9.6E+01	1.0E+01									18%	-6.8	-7.1	-8.8
sodium dimethyldithiocarbamate	204-876-7	128-04-1	128041	1188	Reach_1105	366	143	0.0												18%	-6.8	-7.1	-8.7
benzyl(3-hydroxyphenacyl)methylammonium chloride	253-197-2	36768-62-4	36768624	2776	Reach_2704	367	156	52.1	8.5E+01	1.3E+05	8.7E+00									18%	-6.8	-7.1	-8.8
2-chloroethyldiethylammonium chloride	600-382-4	103041-38-9	103041389	1357	Reach_4061	368	194	78.0	1.4E-01	2.9E+03	4.0E+01									18%	-6.8	-7.1	-8.8
zinc di(benzothiazol-2-yl) disulphide	205-840-3	155-04-4	155044	5716	Reach_1211	369	398	0.0												18%	-6.8	-7.1	-8.8
2-phosphonobutane-1,2,4-tricarboxylic acid	253-733-5	37971-36-1	37971361	2811	Reach_2713	370	270	90.3	8.1E-09	1.6E+04	2.2E-02	1.57		1.1E-06	1.1E-07	3.5E-07				14%	-5.9	-7.1	-9.2
N,N'-bis(2,2,6,6-tetramethylpiperidin-4-yl)hexane-1,6-diamine	262-679-1	61260-55-7	61260557	3330	Reach_2849	371	395	192.6	1.9E-05	2.8E+01	2.7E+04		3.47	3.5E-07	3.5E-08	1.1E-07				18%	-6.6	-7.1	-8.8
sodium toluene-4-sulphonate	211-522-5	657-84-1	657841	5976	Reach_1490	372	194	0.0												18%	-6.8	-7.1	-8.8
octamethylcyclotetrasiloxane	209-136-7	556-67-2	556672	705	Reach_1368	373	297	1.8	1.6E+02	1.3E+00	6.2E+06			7.9E-09	3.5E-09	3.5E-09				24%	-7.4	-7.1	-9.6
dodecanedioic acid	211-746-3	693-23-2	693232	3538	Reach_1506	374	230	142.7	2.6E-04	6.5E+01	1.5E+03	4.6		1.1E-06	1.1E-07	3.5E-07				14%	-6.6	-7.1	-9.1
choline chloride	200-655-4	67-48-1	67481	1231	Reach_81	375	140	0.0												18%	-6.8	-7.1	-8.8
2',4'-dimethylacetoacetanilide	202-576-0	97-36-9	97369	4163	Reach_477	376	205	137.6	1.1E-03	7.5E+02	3.5E+01	10.7	13.4	3.5E-07	3.5E-08	1.1E-07				16%	-6.3	-7.1	-9.0
decamethylcyclopentasiloxane	208-764-9	541-02-6	541026	3125	Reach_1338	377	371	-5.2	2.9E+01	4.8E-02	8.5E+07			3.5E-09	3.5E-09	3.5E-09				24%	-7.3	-7.1	-9.0
2,4-dichloroaniline	607-327-3	24131-07-5	24131075	2375	Reach_4238	378	203	79.0	3.7E-02	1.9E+02	1.3E+02			1.1E-06	1.1E-07	3.5E-07				23%	-6.4	-7.1	-8.1
sodium 2-methylpropan-2-olate	212-741-9	865-48-5	865485	6066	Reach_1570	379	96	0.0												18%	-6.8	-7.1	-8.8
1-(2-butoxy-1-methylethoxy)propan-2-ol	249-951-5	29911-28-2	29911282	2578	Reach_2637	380	190	18.0	4.8E-01	2.7E+05	1.3E+01	15		1.1E-06	1.1E-07	3.5E-07				14%	-6.4	-7.1	-9.2
5-chloro-2-(2,4-dichlorophenoxy)aniline	206-017-1	288-13-1	288131	43	Reach_1223	381	68	-0.3	3.3E+01	4.2E+05	1.1E+00		11.5	4.0E-07	3.5E-08	1.1E-07				14%	-6.6	-7.1	-9.3
5,5-dimethylcyclohexane-1,3-dione	204-804-4	126-81-8	126818	408	Reach_1090	382	140	40.6	6.3E-01	5.8E+04	2.0E+01	5.4		1.4E-07	3.5E-07	1.1E-06				18%	-6.7	-7.1	-8.7
1-chloro-2,4-dinitrobenzene	202-551-4	97-00-7	97007	1056	Reach_476	383	203	93.1	6.5E-02	5.9E+01	1.9E+02			3.2E-08	3.5E-08	1.1E-07				21%	-7.4	-7.1	-8.3
oct-1-ene	203-893-7	111-66-0	111660	1553	Reach_864	384	112	-69.8	2.2E+03	1.0E+01	1.3E+04			1.1E-06	1.1E-07	3.5E-07				21%	-7.4	-7.1	-10.1
2-methyl-4,6-dinitro-phenol	604-165-5	139893-43-9	139893439	5688	Reach_4143	385	454	0.0												23%	-6.7	-7.1	-8.1
2-[(2-methoxy-4-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxol	228-768-4	6358-31-2	6358312	3407	Reach_2168	386	386	241.6	4.3E-10	8.0E+00	9.8E+02	8.66	14.1	3.5E-07	3.5E-08	1.1E-07				16%	-6.3	-7.1	-8.9
triethyl phosphite	204-552-5	122-52-1	122521	1751	Reach_1030	387	166	-21.4	3.7E+02	1.7E+09	5.5E+00			3.5E-07	1.1E-07	3.5E-07				16%	-6.3	-7.1	-9.0
1H-1,2,4-triazole, sodium salt	255-280-9	41253-21-8	41253218	5878	Reach_2741	388	91	0.0												18%	-6.9	-7.1	-8.8
616-083-7	617-435-2	83066-88-0	83066880	950	Reach_4461	389	327	162.8	3.7E-05	5.6E+01	3.8E+03	3.09	13	2.2E-09	1.1E-07	1.1E-06				21%	-6.9	-7.1	-8.4
α,α,α-trifluoro-m-toluidine	202-643-4	98-16-8	98168	1068	Reach_501	390	161	9.6	9.1E+01	4.4E+03	1.1E+02		11	2.1E-08	3.5E-07	1.1E-06				22%	-6.9	-7.1	-8.3
isoprene	201-143-3	78-79-5	78795	900	Reach_209	391	68	-118.9	7.3E+04	5.5E+02	3.8E+02			2.9E-08	1.1E-07	3.5E-07				23%	-7.5	-7.1	-9.9
sebacic acid, compound with hexane-1,6-diamine (1:1)	229-177-4	6422-99-7	6422997	5966	Reach_2183	392	318	0.0												18%	-6.8	-7.1	-8.8
tributyl O-acetylcitrate	201-067-0	77-90-7	77907	3744	Reach_188	393	402	94.4	6.1E-04	3.9E+00	1.9E+04			3.5E-07	3.5E-08	1.1E-07				18%	-7.4	-7.1	-8.9
2,2-dimethylbutyric acid	209-674-2	590-19-2	590192	3264	Reach_1387	394	54	-117.9	1.7E+05	3.3E+03	1.1E+02			1.1E-06	1.1E-07	3.5E-07				23%	-7.3	-7.1	-8.1
sodium 3-(allyloxy)-2-hydroxypropanesulphonate	258-004-5	52556-42-0	52556420	5912	Reach_2782	395	218	0.0												18%	-6.8	-7.2	-8.8
[2-(2-methoxymethylethoxy)methylethoxy]propanol	247-045-4	25498-49-1	25498491	2436	Reach_2569	396	206	25.4	7.1E-01	2.0E+04	6.3E-01	14.9		3.5E-07	1.1E-07	3.5E-07				16%	-7.2	-7.2	-9.0
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	223-861-6	4098-71-9	4098719	2867	Reach_2013	397	222	86.5	1.5E-01	4.5E+02	5.6E+04			1.1E-06	3.5E-07	1.1E-06				17%	-7.3	-7.2	-8.9
1,1,2-trichloroethane	201-166-9	79-00-5	79005	908	Reach_222	398	133	-62.6	2.7E+03	5.0E+03	1.0E+02			2.2E-08	1.1E-08	3.5E-08				23%	-7.5	-7.2	-9.1
Phenol, 4-nonyl-, branched	284-325-5	84852-15-3	84852153	964	Reach_2979	399	220	89.9	8.0E-03	2.5E-01	8.3E+05	10		9.9E-09	1.1E-07	3.5E-07				23%	-7.3	-7.2	-8.3
1,3-dihydro-5-nitro-2H-benzimidazol-2-one	239-743-2	15667-63-7	15667637	2049	Reach_2392	400	125	-157.5	1.6E+03	1.4E+04	1.5E+00			3.5E-06	3.5E-07	1.1E-06				14%	-6.2	-7.2	-9.3
2-propylheptan-1-ol	233-126-1	10042-59-8	10042598	1306	Reach_2278	401	158	-2.8	3.4E+00	4.9E+01	5.1E+03	15.9		1.1E-06	1.1E-07	3.5E-07				16%	-7.4	-7.2	-8.6
N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine	212-344-0	793-24-8	793248	3771	Reach_1548	402	268	121.5	6.6E-04	1.0E+00	4.8E+04		9.4	3.5E-06	1.1E-07	3.5E-07				14%	-6.6	-7.2	-9.2
uronium hydrogen sulphate	244-343-6	21351-39-3	21351393	1205	Reach_2505	403	158	0.0												18%	-6.9	-7.2	-8.8
3,4,5,6-tetrachloro-N-[2-(4,5,6,7-tetrachloro-2,3-dihydro-1,3-d	250-063-5	30125-47-4	30125474	2587	Reach_2643	404	694	349.8	2.3E-19	1.4E-07	1.5E+10	9.55	12.5	3.5E-09	3.5E-09	3.5E-09				23%	-7.0	-7.2	-8.1
docosan-1-ol	211-546-6	661-19-8	661198	3464	Reach_1491	405	327	122.9	8.2E-06	2.8E-04	4.8E+09	15.9		1.1E-06	3.5E-07	1.1E-06				23%	-7.0	-7.2	-7.7
2-diethylaminoethanol	202-845-2	100-37-8	100378	123	Reach_553	406	117	-15.6	8.6E+01	4.0E+05	1.1E+00	15	4	7.8E-08	1.1E-06	3.5E-06				19%	-7.4	-7.2	-8.6
4-nitroaniline	201-208-6	79-44-7	79447	3777	Reach_246	407	108	-15.9	2.4E+02	1.8E+05	1.9E-01		14.4	1.1E-06	1.1E-07	3.5E-07				23%	-6.8	-7.2	-8.1
617-435-2	616-083-7	74351-78-3	74351783	3634	Reach_4422	408	669	349.8	3.7E-22	1.3E-03	1.0E+05	3.55	13.3	3.5E-08	1.1E-08	3.5E-08				23%	-7.1	-7.2	-8.1
dimethyl carbonate	210-478-4	616-38-6	616386	3345	Reach_1431	409	90	-120.1	7.5E+03	1.2E+05	1.7E+00			1.1E-06	3.5E-07	1.1E-06				15%	-7.4	-7.2	-8.6
neodecanoic acid	248-093-9	26896-20-8	26896208	2491	Reach_2595	410	172	48.1	2.0E+00	7.2E+01	6.8E+03	4.9		3.5E-06	3.5E-07	1.1E-06				14%	-7.4	-7.2	-9.1
12-hydroxystearic acid	203-366-1	106-14-9	106149	1429	Reach_656	411	300	152.9	4.5E-07	1.1E+00	2.6E+06	4.9		1.1E-06	1.1E-07	3.5E-07				15%	-6.5	-7.2	-9.0
diuron (reach)	206-354-4	330-54-1	330541	46	Reach_1238	412	233	126.4	6.2E-04	6.4E+01	4.7E+02	13.8	15.6	9.0E-09	3.5E-08	1.1E-07				23%	-6.8	-7.2	-8.2
salicylic acid	200-712-3	69-72-7	69727	84	Reach_95	413	138	93.8	4.3E-03	5.1E+03	1.7E+02	3		1.6E-06	3.5E-07	1.1E-06				14%	-6.6	-7.2	-9.1
N-butylbenzenesulphonamide	222-823-6	3622-84-2	3622842	2763	Reach_1977	414	213	108.0	1.9E-02	1.1E+03	2.0E+02	10.1		3.5E-07	3.5E-08	1.1E-07				16%	-7.2	-7.2	-9.0
N-carboxymethyliminobis(ethylenenitrilo)tetra(acetic acid)	200-652-8	67-43-6	67436	82	Reach_80	415	393	334.2	1.6E-14	2.0E+00	1.2E-05	0.98	2.93	8.8E-08	1.1E-07	3.5E-07				19%	-6.2	-7.2	-8.7
4-aminophenol	204-616-2	123-30-8	123308	386	Reach_1044	416	109	53.6	4.4E-03	2.2E+04	1.7E+00	10.4	9	5.2E-07	1.1E-07	1.1E-06				15%	-6.3	-7.2	-9.1
calcium 4-[(5-chloro-4-methyl-2-sulphonatophenyl)azo]-3-hydr	230-303-5	7023-61-2	7023612	6004	Reach_2220	417	459	0.0												18%	-6.9	-7.2	-8.9
612-012-9	205-334-2	138-59-0	138590	445	Reach_1141	418	174	133.2	6.7E-07	9.6E+04	4.6E-02	4.12		5.9E-07	3.5E-07	1.1E-06				21%	-7.0	-7.2	-8.5
4-[(2,5-dichlorophenyl)azo]-3-hydroxy-2-naphthoic acid	237-913-0	14064-10-9	14064109	450	Reach_2356	419	195	-66.6	1.6E+01	2.3E+03	1.2E+01	6.19		3.1E-07	3.5E-07	1.1E-06				21%	-7.1	-7.2	-8.5
2-ethylhexyl acrylate	203-080-7	103-11-7	103117	159	Reach_602	420	184	-10.4	2.4E+01	5.7E+01	1.2E+04			2.6E-07	3.5E-07	1.1E-06				19%	-7.5	-7.2	-9.0
ethylene carbonate	202-510-0	96-49-1	96491	4149	Reach_467	421	88	12.9	2.9E+00	1.0E+05	4.6E-01			1.1E-06	1.1E-07	3.5E-07				14%	-6.9	-7.2	-9.3
tetramethylsilane	200-899-1	75-76-3	75763	3685	Reach_160	422	88	-116.5	9.5E+04	2.7E+02	5.2E+02			3.5E-09	3.5E-09	3.5E-09				24%	-7.8	-7.2	-10.0
sodium methanethiolate	225-969-9	5188-07-8	5188078	5582	Reach_2084	423	70	0.0												18%	-6.9	-7.2	-8.8
(R)-lactic acid	245-247-7	22818-40-2	22818402	2339	Reach_2524	424	167	238.8	5.9E-06	4.8E+03	5.6E-03	1.99		3.5E-06	3.5E-07	1.1E-06				15%	-6.2	-7.2	-9.1
2-chlorobenzaldehyde	201-956-3	89-98-5	89985	997	Reach_355	425	141	8.7	2.6E+01	9.5E+02	2.2E+02			4.9E-08	1.1E-07	3.5E-07				21%	-7.5	-7.2	-8.5
isooctene	234-294-9	11071-47-9	11071479	1529	Reach_2303	426	112	-81.5	3.3E+03	5.4E+00	1.1E+04			1.1E-06	1.1E-07	3.5E-07				21%	-7.5	-7.2	-10.2
dodecamethylcyclohexasiloxane	208-762-8	540-97-6	540976	3124	Reach_1337	427	445	-8.7	4.7E+00	1.7E-03	1.2E+09			3.5E-09	3.5E-09	3.5E-09				24%	-7.4	-7.2	-8.4

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
[ethylenebis[nitrilobis(methylene)]]tetrakisphosphonic acid, ca	287-370-9	85480-89-3	85480893	6060	Reach_2985	428	499	0.0												18%	-6.9	-7.2	-8.9
ethyl acrylate	205-438-8	140-88-5	140885	452	Reach_1151	429	100	-70.7	5.1E+03	1.6E+04	1.7E+01			3.2E-07	3.5E-07	1.1E-06				17%	-7.5	-7.2	-8.9
chlorodifluoromethane	200-871-9	75-45-6	75456	3673	Reach_145	430	86	-139.4	8.8E+05	1.9E+03	7.8E+00			3.5E-08	1.1E-08	1.1E-08				23%	-7.9	-7.2	-10.0
phenazone	200-486-6	60-80-0	60800	74	Reach_59	431	188	119.2	3.7E-02	4.2E+05	3.9E+00		12.2	4.1E-09	1.1E-07	1.1E-06				23%	-6.8	-7.2	-8.2
disodium phthalate	240-106-6	15968-01-1	15968011	5728	Reach_2406	432	210	0.0												18%	-6.9	-7.2	-8.9
2-pyridylamine	207-988-4	504-29-0	504290	658	Reach_1304	433	94	26.8	1.3E+01	1.6E+04	3.4E+00		7	2.2E-09	1.1E-07	3.5E-07				23%	-7.5	-7.2	-8.1
603-434-4	203-729-4	110-02-1	110021	272	Reach_801	434	84	-45.7	9.8E+03	1.9E+03	6.5E+01			3.0E-08	3.5E-08	1.1E-07				21%	-7.1	-7.2	-8.5
cyclohexyl phenyl ketone	211-923-5	712-50-5	712505	818	Reach_1520	435	188	50.5	2.7E-01	1.0E+01	8.7E+03			1.8E-08	3.5E-07	1.1E-06				23%	-7.5	-7.2	-8.5
tetrasodium 4,4'-{ethene-1,2-diylbis[(3-sulfonato-4,1-phenylen	218-414-7	2146-71-6	2146716	2295	Reach_1764	436	226	23.7	7.1E-01	3.8E+00	4.4E+05									18%	-6.9	-7.2	-8.9
hexane-1,6-diol	211-074-0	629-11-8	629118	3385	Reach_1464	437	118	14.4	1.7E-01	3.4E+05	5.8E+00	15.6		3.5E-06	1.1E-06	3.5E-06				14%	-6.5	-7.2	-9.1
2,3-xylidine	617-346-9	82543-15-5	82543155	3828	Reach_4454	438	316	177.1	5.1E-08	8.6E+02	9.8E+01			1.1E-06	3.5E-07	1.1E-06				23%	-7.5	-7.2	-8.1
biphenyl-4-ol	202-179-2	92-69-3	92693	1013	Reach_388	439	170	86.6	2.3E-03	2.0E+02	1.9E+03	9.2		5.1E-08	3.5E-08	3.5E-08				21%	-7.1	-7.2	-8.6
N-ethylaniline	203-135-5	103-69-5	103695	162	Reach_611	440	121	-9.0	4.1E+01	1.5E+03	1.3E+02		9	6.0E-09	1.1E-07	3.5E-07				23%	-7.5	-7.2	-8.2
cycloheptapentylose	231-493-2	7585-39-9	7585399	6405	Reach_2263	441	1137	0.0												18%	-6.9	-7.2	-8.9
lactonitrile	201-163-2	78-97-7	78977	3762	Reach_220	442	71	-29.2	2.7E+01	1.5E+06	6.5E-02	11		1.1E-06	3.5E-07	1.1E-06				14%	-6.9	-7.2	-9.3
Disodium 4-amino-3-[{4-[({4-[(2,4-diaminophenyl)diazenyl]phe	605-104-5	157577-99-6	157577996	5722	Reach_4167	443	861	0.0												18%	-6.9	-7.2	-8.9
allyl alcohol	203-470-7	107-18-6	107186	213	Reach_697	444	58	-76.4	3.1E+03	4.5E+05	1.6E+00	15.5		4.3E-06	3.5E-07	1.1E-06				14%	-7.5	-7.2	-9.0
2-methoxy-1-methylethyl acetate	203-603-9	108-65-6	108656	1487	Reach_750	445	132	-50.3	6.7E+02	6.9E+04	3.3E+00			3.5E-06	3.5E-07	1.1E-06				14%	-7.5	-7.2	-9.0
3-aminopropyldimethylamine	203-680-9	109-55-7	109557	1503	Reach_777	446	102	-23.3	1.2E+03	4.4E+05	3.5E-01		3.7	3.5E-06	3.5E-07	1.1E-06				14%	-7.5	-7.2	-9.1
thymol	224-832-0	4511-42-6	4511426	2938	Reach_2045	447	144	26.1	2.1E-02	1.5E+07	4.5E+01			3.5E-06	3.5E-07	1.1E-06				22%	-7.5	-7.2	-8.4
disodium 2,2'-([1,1'-biphenyl]-4,4'-diyldivinylene)bis(benzenesu	248-421-0	27344-41-8	27344418	1212	Reach_2602	448	563	0.0												18%	-6.9	-7.3	-8.9
sodium O-ethyl dithiocarbonate	205-440-9	140-90-9	140909	1196	Reach_1153	449	144	0.0												18%	-7.0	-7.3	-8.9
propazine (reach)	205-359-9	139-40-2	139402	446	Reach_1144	450	230	115.7	9.7E-04	6.4E+00	1.7E+03		12	2.2E-09	3.5E-08	1.1E-07				23%	-7.0	-7.3	-8.2
trisodium 2-(carboxylatomethyl(2-hydroxyethyl)amino)ethylim	205-381-9	139-89-9	139899	5689	Reach_1145	451	344	0.0												18%	-6.9	-7.3	-8.9
L-Cysteine, hydrochloride, hydrate	615-117-8	7048-04-6	7048046	5585	Reach_4410	452	158	0.0												18%	-7.0	-7.3	-8.9
sodium sulphanilate	208-208-5	515-74-2	515742	5906	Reach_1319	453	195	0.0												18%	-7.0	-7.3	-8.9
triacetin	203-051-9	102-76-1	102761	1352	Reach_597	454	218	-37.3	7.0E-01	2.5E+04	2.3E+00			3.5E-06	3.5E-07	1.1E-06				14%	-7.2	-7.3	-9.3
potassium (R)-[(3-ethoxy-1-methyl-3-oxoprop-1-enyl)amino]ph	213-510-5	961-69-3	961693	6093	Reach_1620	455	301	0.0												18%	-7.0	-7.3	-8.9
2-(2-butoxyethoxy)ethyl acetate	204-685-9	124-17-4	124174	1787	Reach_1071	456	204	23.9	4.7E+00	7.5E+03	2.0E+01			1.1E-06	3.5E-07	1.1E-06				14%	-7.5	-7.3	-9.1
ethylamine	200-834-7	75-04-7	75047	846	Reach_125	457	45	-84.9	2.0E+04	1.0E+06	7.1E-01		4	4.1E-07	3.5E-07	1.1E-06				16%	-7.5	-7.3	-8.5
2-(2-(2-butoxyethoxy)ethoxy)ethanol	205-592-6	143-22-6	143226	1959	Reach_1190	458	206	56.4	6.9E-02	1.2E+06	1.0E+00	14.9		1.1E-06	1.1E-07	3.5E-07				14%	-6.3	-7.3	-9.4
4-methyloxazole-5-carbonitrile	214-029-3	1073-69-4	1073694	1461	Reach_1643	459	143	44.2	5.9E+00	9.9E+04	2.8E+01		9	3.5E-07	1.1E-07	3.5E-07				14%	-6.2	-7.3	-9.3
octadec-1-ene	204-012-9	112-88-9	112889	1609	Reach_928	460	252	29.6	3.5E-01	6.8E-04	1.1E+09			1.1E-06	1.1E-07	3.5E-07				23%	-7.2	-7.3	-8.8
2-(dimethylamino)ethyl acrylate	219-460-0	2439-35-2	2439352	2391	Reach_1811	461	143	-23.6	2.3E+02	3.0E+04	2.6E+00		5.8	3.5E-06	3.5E-07	1.1E-06				14%	-7.5	-7.3	-9.0
4,4'-methylenebis[2-chloroaniline]	202-918-9	101-14-4	101144	1315	Reach_573	462	267	156.6	5.2E-04	7.7E+00	3.0E+03		10.7	3.5E-07	1.1E-08	3.5E-08				16%	-6.7	-7.3	-9.2
γ-butyrolactone	202-509-5	96-48-0	96480	4148	Reach_466	463	86	-42.1	3.9E+01	8.3E+04	4.9E-01			3.5E-06	3.5E-07	1.1E-06				14%	-7.5	-7.3	-9.3
disodium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4-)-M	237-864-5	14025-15-1	14025151	1193	Reach_2354	464	384	0.0												18%	-7.0	-7.3	-8.9
tetrachloroethylene	204-825-9	127-18-4	127184	20	Reach_1096	465	166	-60.6	2.4E+03	4.6E+02	9.3E+02			3.9E-08	3.5E-08	1.1E-07				23%	-7.6	-7.3	-9.7
sodium dihydrogen citrate	242-734-6	18996-35-5	18996355	5752	Reach_2473	466	214	0.0												18%	-7.0	-7.3	-8.9
2,2',6,6'-Tetrabromo-4,4'-isopropylidenediphenol, oligomeric r	500-107-7	40039-93-8	40039938	5873	Reach_4053	467	636	0.0												18%	-7.0	-7.3	-9.0
sodium 2-ethylhexanoate	243-283-8	19766-89-3	19766893	5763	Reach_2484	468	166	0.0												18%	-7.0	-7.3	-8.9
2-methoxyethanol	203-713-7	109-86-4	109864	267	Reach_794	469	76	-56.6	7.5E+02	8.8E+05	1.2E-01	15		1.5E-06	3.5E-07	1.1E-06				14%	-7.5	-7.3	-9.2
zirconium acetate	231-492-7	7585-20-8	7585208	6028	Reach_2262	470	327	0.0												18%	-7.0	-7.3	-8.9
hexasodium 2,2'-[vinylenebis[(3-sulphonato-4,1-phenylene)imi	273-468-9	68971-49-3	68971493	6000	Reach_2914	471	1369	0.0												18%	-7.0	-7.3	-9.0
zinc bis(dibenzyldithiocarbamate)	238-778-0	14726-36-4	14726364	5701	Reach_2368	472	610	0.0												18%	-7.0	-7.3	-9.0
carbon disulphide	200-843-6	75-15-0	75150	852	Reach_132	473	76	-77.0	4.6E+04	3.9E+03	8.7E+01			2.9E-09	3.5E-07	1.1E-06				24%	-7.6	-7.3	-9.7
pentaerithrityl tetranitrate	201-084-3	78-11-5	78115	892	Reach_194	474	316	119.5	5.6E-04	6.3E+03	2.4E+02			1.7E-07	3.5E-08	1.1E-07				18%	-6.6	-7.3	-9.0
diammonium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]]((	270-232-7	68413-60-5	68413605	5997	Reach_2906	475	397	0.0												18%	-7.0	-7.3	-9.0
ethylenediaminetetraacetonitrile	227-290-3	5766-67-6	5766676	3236	Reach_2135	476	216	159.5	2.2E-05	1.0E+06	6.8E-03			3.5E-07	1.1E-07	3.5E-07				16%	-6.3	-7.3	-9.2
sodium O-isobutyl dithiocarbonate	246-805-2	25306-75-6	25306756	1209	Reach_2564	477	172	0.0												18%	-7.0	-7.3	-8.9
chlorotrimethylsilane	200-900-5	75-77-4	75774	3686	Reach_161	478	109	-103.3	2.6E+04	1.4E+03	3.0E+02			3.5E-09	3.5E-09	3.5E-09				24%	-7.9	-7.3	-10.0
toluenesulphonamide	215-578-1	1333-07-9	1333079	1866	Reach_1678	479	171	91.2	8.1E-03	2.3E+03	8.3E+00	10.1		3.5E-07	3.5E-08	1.1E-07				16%	-6.7	-7.3	-9.2
sodium prop-2-enesulphonate	219-676-5	2495-39-8	2495398	5793	Reach_1823	480	144	0.0												18%	-7.0	-7.3	-9.0
5H-dibenz[b,f]azepine	209-798-7	593-56-6	593566	1226	Reach_1394	481	84	0.0												16%	-7.0	-7.3	-9.2
1,2,4-triazole	206-022-9	288-88-0	288880	584	Reach_1224	482	69	21.6	8.0E+01	1.6E+05	1.7E-01	10.5	12	8.1E-07	3.5E-08	1.1E-07				15%	-6.3	-7.3	-9.4
[nitrilotris(methylene)]trisphosphonic acid, sodium salt	243-900-0	20592-85-2	20592852	2271	Reach_2496	483	299	90.3	2.7E-09	1.0E+06	3.5E-06	2.29	3.11	3.5E-07	3.5E-08	1.1E-07				16%	-6.2	-7.3	-9.2
butene	246-689-3	25167-67-3	25167673	2419	Reach_2560	484	56	-121.7	2.5E+05	1.1E+03	1.5E+02			1.1E-06	1.1E-07	3.5E-07				20%	-7.6	-7.3	-10.3
2-amino-4,5-dichlorobenzenesulfonic acid	700-372-0	1128026-41-4	1128026414	1604	Reach_4877	485	311	53.4	2.9E-01		1.4E+03			1.1E-06	1.1E-07	1.1E-06				19%	-6.3	-7.3	-8.9
m-xylene	203-576-3	108-38-3	108383	236	Reach_742	486	106	-40.7	8.8E+02	1.9E+02	1.2E+03			5.7E-07	3.5E-08	1.1E-07				20%	-7.6	-7.3	-9.7
4-chlorobenzonitrile	244-870-1	22252-43-3	22252433	2326	Reach_2520	487	214	298.1	1.1E-07	8.4E+03	1.3E-01			1.1E-06	1.1E-07	3.5E-07				23%	-7.6	-7.3	-8.4
diguanidinium carbonate	209-813-7	593-85-1	593851	5942	Reach_1397	488	180	0.0												18%	-7.0	-7.3	-9.0
6-hydroxy-1H-pyrimidin-4-one	214-772-3	1193-24-4	1193244	1690	Reach_1671	489	112	83.3	2.3E-01	6.7E+04	3.0E+00	5.4		3.5E-07	1.1E-07	3.5E-07				16%	-6.4	-7.3	-9.2
4-amino-2,5-dichlorobenzenesulphonic acid	263-560-7	62476-59-9	62476599	1228	Reach_2853	490	384	0.0												19%	-6.3	-7.3	-8.9
nicotinamide	202-713-4	98-92-0	98920	1079	Reach_524	491	122	99.4	2.6E-02	1.8E+05	3.5E-01	14.8	11	2.3E-07	1.1E-07	3.5E-07				17%	-6.4	-7.3	-9.1
potassium mercaptoacetate	252-038-4	34452-51-2	34452512	5852	Reach_2679	492	130	0.0												18%	-7.0	-7.3	-9.0
2-ethylhexyl nitrate	248-363-6	27247-96-7	27247967	2497	Reach_2599	493	175	-15.0	3.5E+01	1.7E+02	1.3E+04			1.1E-06	1.1E-07	3.5E-07				16%	-7.6	-7.3	-9.0
ammonium mercaptoacetate	226-540-9	5421-46-5	5421465	5923	Reach_2109	494	109	0.0												18%	-7.0	-7.3	-9.0
(methoxymethyl)triphenylphosphonium chloride	204-077-3	115-27-5	115275	1635	Reach_941	495	371	129.6	8.6E-05	7.1E-01	2.3E+04									18%	-7.0	-7.3	-9.0
2-isopropoxyethanol	203-685-6	109-59-1	109591	257	Reach_778	496	104	-43.5	2.4E+02	2.5E+05	1.0E+00	15		4.3E-09	3.5E-07	1.1E-06				23%	-7.6	-7.3	-8.4
2,2,6,6-tetramethyl-4-piperidone	212-554-2	826-36-8	826368	3834	Reach_1556	497	155	53.1	2.7E+01	3.2E+03	2.7E+00		4.2	1.1E-06	3.5E-07	1.1E-06				14%	-7.6	-7.3	-8.9
biphenyl-4,4'-diol	202-200-5	92-88-6	92886	1015	Reach_395	498	186	127.0	1.5E-06	2.2E+02	6.3E+02	8.89		6.9E-08	3.5E-08	3.5E-08				20%	-6.6	-7.3	-8.8
1,2-dichloropropane	201-152-2	78-87-5	78875	902	Reach_213	499	113	-79.7	6.1E+03	3.1E+03	1.8E+02			1.0E-08	1.1E-08	3.5E-08				23%	-7.7	-7.3	-9.5
barium bis[2-chloro-5-[(2-hydroxy-1-naphthyl)azo]toluene-4-su	225-935-3	5160-02-1	5160021	5581	Reach_2081	500	889	0.0												18%	-7.0	-7.3	-9.0
2-butene	203-452-9	107-01-7	107017	1454	Reach_689	501	56	-120.4	2.3E+05	9.3E+02	1.2E+02			3.5E-06	3.5E-07	1.1E-06				17%	-7.7	-7.3	-10.6
ametryn (reach)	212-634-7	834-12-8	834128	953	Reach_1562	502	227	130.6	5.7E-03	1.8E+02	2.1E+03		10	2.2E-09	1.1E-07	1.1E-07				23%	-7.1	-7.3	-8.3

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
methyltriphenylphosphonium bromide	201-056-0	77-76-9	77769	3735	Reach_184	503	104	-75.5	1.1E+04	2.8E+04	2.4E+01									18%	-7.0	-7.3	-9.0
cyclohex-1,2-ylenediamine	211-776-7	694-83-7	694837	807	Reach_1510	504	114	27.0	5.4E+01	1.0E+06	1.2E+00		4	4.2E-08	3.5E-07	3.5E-07				21%	-7.5	-7.3	-8.6
2-methylpropan-1-ol	201-148-0	78-83-1	78831	901	Reach_210	505	74	-74.0	1.8E+03	1.0E+05	5.9E+00	15.9		4.3E-06	1.1E-06	3.5E-06				14%	-7.6	-7.3	-9.0
benzene-1,2,4-tricarboxylic acid 1,2-anhydride	209-008-0	552-30-7	552307	3164	Reach_1358	506	192	118.1	7.6E-05	4.1E+02	8.9E+01	3.35		3.5E-06	3.5E-07	1.1E-06				14%	-6.6	-7.3	-9.3
[ethylenebis[nitrilobis(methylene)]]tetrakisphosphonic acid, so	244-742-5	22036-77-7	22036777	5776	Reach_2513	507	524	0.0												18%	-7.0	-7.3	-9.0
Amines, bis(hydrogenated tallow alkyl), 2-[[bis(hydrogenated t	294-705-2	91745-35-6	91745356	6407	Reach_2995	508	1191	0.0												18%	-7.0	-7.3	-9.0
sodium decyl sulphate	205-568-5	142-87-0	142870	5696	Reach_1182	509	260	0.0												18%	-7.0	-7.4	-9.0
ammonium myristate	240-599-8	16530-71-5	16530715	5734	Reach_2424	510	245	0.0												18%	-7.0	-7.4	-9.0
dioctadecyl 3,3'-thiodipropionate	211-750-5	693-36-7	693367	3539	Reach_1507	511	683	272.5	5.3E-13	2.4E-12	4.8E+17			1.1E-06	1.1E-07	3.5E-07				24%	-7.6	-7.4	-5.5
Castor oil, hydrogenated, lithium salt	265-222-4	64754-95-6	64754956	6402	Reach_2866	512	945	0.0												18%	-7.0	-7.4	-9.0
methyl acrylate	202-500-6	96-33-3	96333	1053	Reach_462	513	86	-83.5	1.2E+04	3.3E+04	5.4E+00			3.2E-07	3.5E-07	1.1E-06				17%	-7.6	-7.4	-9.0
potassium sulphanilate	213-834-7	1025-15-6	1025156	1343	Reach_1635	514	249	194.9	3.3E-05	9.2E+02	1.3E+05									18%	-7.1	-7.4	-9.0
4,5,6,7-tetrahydrothieno[3,2-c]pyridinium chloride	246-073-4	24199-46-0	24199460	2376	Reach_2540	515	140	-28.3	1.4E+02	1.0E+03	3.5E+02									18%	-7.1	-7.4	-9.0
disodium [N,N-bis[2-[bis(carboxymethyl)amino]ethyl]glycinato(	243-136-8	19529-38-5	19529385	5762	Reach_2481	516	495	0.0												18%	-7.0	-7.4	-9.0
butanone oxime	202-496-6	96-29-7	96297	1051	Reach_459	517	87	-58.0	1.6E+02	2.2E+04	4.9E+01	12.5		2.7E-07	1.1E-07	3.5E-07				17%	-7.6	-7.4	-8.7
piperazine	203-808-3	110-85-0	110850	1531	Reach_832	518	86	7.3	9.5E+01	1.0E+06	1.6E-01		4.4	3.5E-06	3.5E-07	1.1E-06				14%	-7.4	-7.4	-9.5
N-butyl-2,2,6,6-tetramethylpiperidin-4-amine	252-899-6	36177-92-1	36177921	2761	Reach_2698	519	212	80.0	2.0E-01	3.6E+03	7.6E+02		3.75	3.5E-07	1.1E-07	3.5E-07				16%	-7.6	-7.4	-9.1
docosyltrimethylammonium methyl sulphate	279-791-1	81646-13-1	81646131	6043	Reach_2960	520	480	0.0												18%	-7.1	-7.4	-9.0
2,2'-methyliminodiethanol	203-312-7	105-59-9	105599	1416	Reach_645	521	119	24.9	3.3E-01	1.0E+06	3.2E-02	14.7	5	3.5E-06	1.1E-06	3.5E-06				14%	-6.5	-7.4	-9.4
trisodium bis[3-hydroxy-4-[(2-hydroxy-1-naphthyl)azo]-7-nitro	260-906-9	57693-14-8	57693148	5938	Reach_2826	522	1004	0.0												18%	-7.0	-7.4	-9.0
stearic acid	200-313-4	57-11-4	57114	3223	Reach_38	523	284	133.0	1.1E-03	2.4E-02	8.7E+07	4.9		1.1E-06	1.1E-07	3.5E-07				18%	-7.5	-7.4	-9.2
2,2'-dimethyl-2,2'-azodipropiononitrile	201-132-3	78-67-1	78671	3754	Reach_203	524	164	43.9	1.9E-01	7.2E+02	7.4E+02			3.5E-07	1.1E-07	3.5E-07				16%	-7.6	-7.4	-9.1
glyoxylic acid	206-058-5	298-12-4	298124	2573	Reach_1228	525	74	16.1	2.5E+01	2.5E+05	4.0E-02	3.5		3.5E-06	3.5E-07	1.1E-06				14%	-6.2	-7.4	-9.4
2,3-dichloropyridine	200-624-5	66-25-1	66251	788	Reach_78	526	100	-55.1	1.3E+03	5.2E+03	6.3E+01			3.9E-06	3.5E-07	1.1E-06				19%	-6.6	-7.4	-9.0
4-chloro-2,5-dimethoxyaniline	228-782-0	6358-64-1	6358641	3409	Reach_2170	527	188	78.6	1.6E-01	1.7E+03	7.6E+01		10.7	1.1E-06	3.5E-07	1.1E-06				14%	-6.7	-7.4	-9.3
sodium 1,4-bis(1,3-dimethylbutyl) sulphonatosuccinate	219-147-9	2373-38-8	2373388	5788	Reach_1789	528	388	0.0												18%	-7.1	-7.4	-9.0
lauric acid	205-582-1	143-07-7	143077	468	Reach_1188	529	200	81.9	1.9E-01	2.7E+01	1.0E+05	4.9		3.7E-06	1.1E-07	3.5E-07				14%	-7.5	-7.4	-9.4
cysteine hydrochloride	200-157-7	52-89-1	52891	5917	Reach_17	530	158	0.0												18%	-7.1	-7.4	-9.0
sodium 3-nitrobenzenesulphonate	204-857-3	127-68-4	127684	5650	Reach_1101	531	225	0.0												18%	-7.1	-7.4	-9.0
allyl 2,3-epoxypropyl ether	203-442-4	106-92-3	106923	201	Reach_682	532	114	-44.5	5.7E+02	6.2E+04	2.8E+00			4.9E-08	1.1E-07	3.5E-07				21%	-7.7	-7.4	-8.6
6-ethyl-2-toluidine	247-323-5	25899-50-7	25899507	2446	Reach_2571	533	81	-46.7	5.4E+02	3.0E+03	1.3E+01			3.5E-07	1.1E-07	3.5E-07				14%	-6.9	-7.4	-9.4
benzenesulphonic acid	202-638-7	98-11-3	98113	4179	Reach_499	534	158	88.8	2.3E-03	7.1E+03	6.8E-02	0.7		3.5E-07	3.5E-08	1.1E-07				16%	-6.3	-7.4	-9.3
1,3-dichloro-4-nitrobenzene	203-687-7	109-61-5	109615	1504	Reach_780	535	123	-56.5	2.6E+03	6.5E+03	1.3E+01			3.5E-06	3.5E-07	1.1E-06				23%	-7.7	-7.4	-8.7
isobutyraldehyde	201-149-6	78-84-2	78842	3759	Reach_211	536	72	-92.1	2.2E+04	7.5E+04	5.5E+00			3.5E-06	1.1E-06	3.5E-06				14%	-7.7	-7.4	-9.1
Ethyl (2S)-2-({[(2-isopropyl-1,3-thiazol-4-yl)methyl](methyl)carb	931-074-0	1247119-36-3	1247119363	5641	Reach_5130	537	503	0.0												18%	-7.1	-7.4	-9.1
2-ethylhexyl oleate	247-655-0	26399-02-0	26399020	2468	Reach_2581	538	395	133.7	2.0E-05	6.0E-06	2.4E+11			1.1E-06	1.1E-07	3.5E-07				24%	-7.6	-7.4	-8.0
propargite	219-006-1	2312-35-8	2312358	548	Reach_1783	539	350	168.8	5.3E-08	8.7E-02	5.2E+04			6.2E-09	1.1E-07	3.5E-07				23%	-6.9	-7.4	-8.4
sodium 4-(4-methyl-3-nitrobenzoylamino)benzenesulphonate	281-719-9	84029-45-8	84029458	6049	Reach_2969	540	358	0.0												18%	-7.1	-7.4	-9.0
bis(2-ethylhexyl) terephthalate	229-176-9	6422-86-2	6422862	3430	Reach_2182	541	391	63.9	2.9E-03	1.0E-02	2.5E+08			1.1E-06	1.1E-07	3.5E-07				23%	-7.2	-7.4	-8.8
[[(phosphonomethyl)imino]bis[ethylenenitrilobis(methylene)]]t	274-798-6	70714-66-8	70714668	6006	Reach_2920	542	590	0.0												18%	-7.1	-7.4	-9.1
sodium (5s,8s)-8-methoxy-2,4-dioxo-1,3-diazaspiro[4.5]decan-	929-513-6	1400584-86-2	1400584862	5690	Reach_5126	543	221	0.0												18%	-7.1	-7.4	-9.0
691-746-1	937-694-8	15295-77-9	15295779	5713	Reach_5145	544	182	0.0												18%	-7.1	-7.4	-9.1
614-977-1	204-973-4	130-00-7	130007	1831	Reach_1115	545	169	142.6	1.1E-04	2.8E+02	1.3E+02									18%	-7.1	-7.4	-9.1
2-(chloromethyl)-3-methyl-4-(2,2,2-trifluoroethoxy)pyridine hy	700-531-4	1093205-93-6	1093205936	1498	Reach_4925	546	275	196.4	4.3E-07	9.6E+00	1.2E+02									18%	-7.1	-7.4	-9.1
N-[2-(3-carbamoyl-4-hydroxyphenyl)-2-oxoethyl]-N-(4-phenylb	700-288-4	96441-14-4	96441144	6094	Reach_4843	547	363	0.0												18%	-7.1	-7.4	-9.1
6,6'-[(3,3'-di-tert-butyl-5,5'-dimethoxybiphenyl-2,2'-diyl)bis(oxy	204-979-7	130-17-6	130176	1833	Reach_1117	548	320	238.4	2.5E-12	1.4E+03	2.6E+00									18%	-7.1	-7.4	-9.1
607-657-8	687-783-8	13222-26-9	13222269	1855	Reach_4637	549	141	-34.6	2.0E+03	2.8E+03	4.5E+00									18%	-7.1	-7.4	-9.1
3-chloropropyldimethylammonium chloride	700-022-7	13349-82-1	13349821	1867	Reach_4127	550	174	89.5	5.2E-03	1.0E+06	1.4E-02									18%	-7.1	-7.4	-9.0
[2-(4-benzyl-2-phenylpiperazin-1-yl)phenyl]methanol (2E)-but-	205-066-6	132-57-0	132570	1860	Reach_1123	551	224	173.0	1.2E-07	4.0E+03	3.4E-01									18%	-7.1	-7.4	-9.1
604-165-5	617-251-2	816431-72-8	816431728	3809	Reach_4448	552	354	229.4	2.8E-09	1.1E+01	5.5E+01									18%	-7.1	-7.4	-9.1
(3aR,8aS,8bS)-1,3-Dibenzyl-2-oxodecahydrothieno[1',2':1,2]thi	286-111-7	85187-23-1	85187231	3884	Reach_2983	553	294	135.6	2.4E-04	2.7E-02	1.0E+06									18%	-7.1	-7.4	-9.1
(2-ethoxy-1-methyl-2-oxoethyl)triphenylphosphonium bromide	211-838-3	700-13-0	700130	3554	Reach_1515	554	152	86.1	2.7E-02	2.1E+03	4.7E+02									18%	-7.1	-7.4	-9.1
methyl (2S-trans)-6,8-dideoxy-6-[[(1-methyl-4-propylpyrrolidin	201-475-9	83-42-1	83421	954	Reach_282	555	172	56.5	5.0E+00	1.1E+02	1.0E+03									18%	-7.1	-7.4	-9.1
disodium 4,4'-methylenebis[3-hydroxy-2-naphthoate]	620-109-2	77820-58-7	77820587	3737	Reach_4558	556	186	74.8	1.5E-01	1.3E+03	8.1E+02									18%	-7.1	-7.4	-9.1
2-chloroethyldimethylammonium chloride	256-350-1	48076-38-6	48076386	2970	Reach_2759	557	353	116.5	1.9E-04	1.7E-05	1.1E+10									18%	-7.1	-7.4	-9.0
611-624-3	241-293-7	17261-28-8	17261288	2129	Reach_2431	558	306	182.0	1.0E-06	1.3E+00	3.6E+04									18%	-7.1	-7.4	-9.1
(2,4-diaminopteridin-6-yl)methanol monohydrochloride	700-274-8	73978-41-3	73978413	6019	Reach_4834	559	229	0.0												18%	-7.1	-7.4	-9.1
(2S)-N-[(diethylamino)methyl]-2-(2-oxopyrrolidin-1-yl)butanam	692-514-2	133047-57-1	133047571	1865	Reach_4676	560	660	349.8	1.5E-25	4.8E-04	6.3E-02									18%	-7.1	-7.4	-9.1
(3S)-N,N-dimethyl-3-(naphthalen-1-yloxy)-3-(thiophen-2-yl)pro	236-412-4	13360-57-1	13360571	1868	Reach_2329	561	144	26.4	5.0E+01	8.5E+04	9.5E+01									18%	-7.1	-7.4	-9.1
Salt of N-acetyl-L-glutamic acid and 1-[(7S)-3,4-dimethoxybicyc	603-772-2	133865-89-1	133865891	1871	Reach_4129	562	302	190.5	1.0E-06	8.4E+00	2.2E+02									18%	-7.1	-7.4	-9.1
N-methylhyoscinium bromide	206-340-8	328-99-4	328994	2667	Reach_1236	563	192	-4.9	1.5E+02	5.6E+02	1.2E+02									18%	-7.1	-7.4	-9.1
hyoscine hydrobromide	619-590-1	135302-13-5	135302135	1888	Reach_4531	564	129	107.1	1.3E-02	1.2E+05	5.8E-02									18%	-7.1	-7.4	-9.1
sodium 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoa	201-920-7	89-58-7	89587	3981	Reach_346	565	151	53.2	6.0E+00	1.2E+02	8.1E+02									18%	-7.1	-7.4	-9.1
692-713-4	619-328-6	98231-71-1	98231711	6095	Reach_4514	566	252	0.0												18%	-7.1	-7.4	-9.1
2-[tert-butyl(phenylmethyl)amino]-1-[4-hydroxy-3-(hydroxyme	619-779-9	120100-77-8	120100778	1704	Reach_4544	567	347	175.3	9.9E-06	4.3E+01	2.7E+01									18%	-7.1	-7.4	-9.1
5-aminopyrazole-4-carboxamide hemisulphate	208-610-0	535-13-7	535137	3105	Reach_1333	568	137	-51.5	6.1E+02	5.0E+03	3.5E+01									18%	-7.1	-7.4	-9.1
1-{[2-(2,4-difluorophenyl)oxiran-2-yl]methyl}-1H-1,2,4-triazole	603-957-8	13636-02-7	13636027	1898	Reach_4134	569	185	69.7	1.7E-02	2.4E+04	1.0E+01									18%	-7.1	-7.4	-9.1
616-640-4	692-713-4	886588-62-1	886588621	6075	Reach_4678	570	380	0.0												18%	-7.1	-7.4	-9.1
(2-carbamimidamido-1,3-thiazol-4-yl)methyl carbamimidothioa	205-289-9	137-32-6	137326	1907	Reach_1138	571	88	-61.5	6.1E+02	3.7E+04	1.8E+01									18%	-7.1	-7.4	-9.1
600-588-4	237-307-6	13734-41-3	13734413	1908	Reach_2347	572	217	88.8	4.2E-02	3.8E+03	7.9E+01									18%	-7.1	-7.4	-9.1
4,4,13,13-tetraethoxy-3,14-dioxa-8,9-dithia-4,13-disilahexadec	260-350-7	56706-10-6	56706106	3209	Reach_2819	573	475	170.8	2.6E-06	7.2E-02	6.0E+03			1.1E-06	1.1E-07	3.5E-07				15%	-7.5	-7.4	-9.3
611-000-0	220-635-9	2840-28-0	2840280	2529	Reach_1874	574	172	114.2	5.2E-04	3.6E+03	4.0E+01									18%	-7.1	-7.4	-9.1
benzyldimethyl[2-[(1-oxoallyl)oxy]ethyl]ammonium chloride	609-118-2	353497-37-7	353497377	2730	Reach_4290	575	281	141.2	1.6E-04	6.2E+00	1.7E+04									18%	-7.1	-7.4	-9.1
619-328-6	700-178-6	121627-17-6	121627176	6393	Reach_4793	576	787	0.0												18%	-7.1	-7.4	-9.1
8-benzyl-3-oxo-8-azoniabicyclo[3.2.1]octane chloride	696-512-2	1378387-81-5	1378387815	1912	Reach_4718	577	420	284.8	9.9E-17	5.8E+04	5.2E-03									18%	-7.1	-7.4	-9.1

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
1-(2-isopropyl-1,3-thiazol-4-yl)-N-methylmethanamine dihydro	604-047-3	137863-20-8	137863208	1913	Reach_4139	578	526	317.9	2.3E-15	7.9E-05	5.2E+05									18%	-7.1	-7.4	-9.1
N,N,N-trimethyladamantan-1-aminium chloride	250-550-2	31291-60-8	31291608	2623	Reach_2653	579	206	76.3	4.2E-02	4.3E+01	2.6E+05									18%	-7.1	-7.4	-9.1
603-758-6	610-029-6	4245-76-5	4245765	2892	Reach_4320	580	118	34.6	1.7E+01	3.7E+05	6.8E-02									18%	-7.1	-7.4	-9.1
617-892-8	212-090-0	761-65-9	761659	871	Reach_1533	581	157	38.0	4.2E+00	3.8E+03	1.0E+02									18%	-7.1	-7.4	-9.1
N-(aminosulfonyl)-3-chloropropanimidamide hydrochloride	604-112-6	139147-73-2	139147732	1917	Reach_4142	582	237	21.9	7.0E+00		6.3E+05									18%	-7.1	-7.4	-9.1
glucosamine hydrochloride	642-256-1	139481-58-6	139481586	1920	Reach_4610	583	469	321.9	1.2E-15	1.2E-03	1.7E+05									18%	-7.1	-7.4	-9.1
Potassium 4-methylbenzenesulfinate	205-410-5	140-29-4	140294	1926	Reach_1148	584	117	9.4	8.7E+00	8.3E+02	3.6E+01									18%	-7.1	-7.4	-9.1
lysine hydrochloride	230-356-4	7065-46-5	7065465	2117	Reach_2221	585	135	-35.5	1.6E+03	3.1E+03	2.4E+01									18%	-7.1	-7.4	-9.1
(3S)-2-Oxotetrahydrofuran-3-ammonium bromide	604-254-9	141818-73-7	141818737	1943	Reach_4145	586	362	201.9	1.9E-07	1.5E+02	9.3E+01									18%	-7.1	-7.4	-9.1
cefazolin	601-332-4	114882-16-5	114882165	1627	Reach_4085	587	355	192.7	8.5E-09	7.4E+00	1.2E+04	11		1.1E-06	1.1E-07	3.5E-07				19%	-6.4	-7.4	-9.0
sodium phenoxyacetate hemihydrate	608-031-7	27006-83-3	27006833	2492	Reach_4259	588	193	72.6	7.4E-01	1.0E+03	1.7E+01									18%	-7.1	-7.4	-9.1
620-019-3	607-957-9	26567-10-2	26567102	2477	Reach_4255	589	242	161.0	2.2E-06	1.5E+00	9.8E+04									18%	-7.1	-7.4	-9.1
metformin hydrochloride	238-056-5	14205-39-1	14205391	1944	Reach_2358	590	115	-19.4	2.9E+02	1.9E+04	5.4E-01									18%	-7.1	-7.4	-9.1
sodium N-methyltaurinate	922-576-0	1184182-45-3	1184182453	5617	Reach_5095	591	400	0.0												18%	-7.1	-7.4	-9.1
hydrogen cyanide	200-821-6	74-90-8	74908	841	Reach_116	592	27	-88.0	9.9E+04	3.4E+04	2.0E-01			6.9E-07	1.1E-07	3.5E-07				16%	-7.8	-7.4	-9.4
609-368-2	618-106-6	88046-01-9	88046019	6074	Reach_4485	593	303	0.0												18%	-7.1	-7.4	-9.1
tert-butylhydrazine monohydrochloride	205-533-4	142-30-3	142303	1953	Reach_1177	594	142	45.1	9.4E-01	3.0E+17	6.5E+00									18%	-7.1	-7.4	-9.1
sulphur dichloride	251-020-3	32388-55-9	32388559	2651	Reach_2661	595	246	91.7	7.6E-02	1.1E+01	1.0E+05									18%	-7.1	-7.4	-9.1
1,2-dichloro-4-nitrobenzene	213-709-7	1003-52-7	1003527	1302	Reach_1634	596	108	15.6	9.6E+01	5.3E+03	2.0E+00			1.1E-06	1.1E-07	3.5E-07				23%	-7.7	-7.4	-8.7
dec-1-ene	212-819-2	872-05-9	872059	3921	Reach_1578	597	140	-45.5	2.8E+02	6.4E-01	1.3E+05			3.5E-07	3.5E-08	1.1E-07				23%	-7.7	-7.4	-10.2
1,1'-isopropylidenebis(p-phenyleneoxy)dipropan-2-ol	204-137-9	116-37-0	116370	1648	Reach_954	598	344	174.6	6.8E-09	2.0E+03	1.1E+04	14.6		3.5E-07	3.5E-08	1.1E-07				17%	-6.7	-7.4	-9.1
didecyldimethylammonium chloride	230-525-2	7173-51-5	7173515	1233	Reach_2228	599	362	0.0												18%	-7.1	-7.4	-9.1
hydroquinone	204-617-8	123-31-9	123319	388	Reach_1045	600	110	45.7	2.2E-03	1.0E+05	1.1E+01	10.1		1.9E-06	3.5E-07	1.1E-06				14%	-6.6	-7.4	-9.4
6-chloro-N,N,N',N'-tetrabutyl-1,3,5-triazine-2,4-diamine	609-724-7	39605-45-3	39605453	2843	Reach_4309	601	370	179.8	5.1E-06	7.1E-03	2.6E+08		12.3	1.1E-07	3.5E-08	1.1E-07				19%	-7.0	-7.4	-9.0
4'-chloro-2-nitrobiphenyl	242-262-0	18379-25-4	18379254	2187	Reach_2460	602	248	-7.5	1.1E+02	1.8E+02	1.8E+05			1.1E-06	3.5E-07	1.1E-06				20%	-7.6	-7.4	-8.9
potassium isopentyl dithiocarbonate	213-180-2	928-70-1	928701	6083	Reach_1601	603	202	0.0												18%	-7.1	-7.4	-9.1
cystine	200-296-3	56-89-3	56893	717	Reach_33	604	240	301.3	3.5E-08	1.2E+03	4.6E-05	1.37	5	3.0E-07	3.5E-07	1.1E-06				16%	-6.3	-7.4	-9.2
bis(2-ethylhexyl) adipate	203-090-1	103-23-1	103231	160	Reach_603	605	371	9.0	4.3E-04	1.5E-02	1.3E+08			4.3E-07	1.1E-07	3.5E-07				23%	-7.2	-7.4	-8.4
thiourea	200-543-5	62-56-6	62566	767	Reach_66	606	76	25.8	7.8E+00	1.0E+06	4.9E-02	13	12	2.7E-09	3.5E-07	1.1E-06				23%	-6.8	-7.4	-8.4
tosyl chloride	202-684-8	98-59-9	98599	4188	Reach_514	607	191	75.3	1.6E-01	2.1E+02	3.1E+03			3.5E-07	3.5E-08	1.1E-07				17%	-7.7	-7.4	-9.1
9-hydroxyandrost-4-ene-3,17-dione	202-440-0	95-68-1	95681	1036	Reach_437	608	121	29.1	2.4E+01	1.0E+03	1.5E+02			2.8E-07	3.5E-08	1.1E-07				16%	-6.5	-7.4	-9.3
2,3-didehydro-3-O-sodio-D-erythro-hexono-1,4-lactone	228-973-9	6381-77-7	6381777	5964	Reach_2175	609	198	0.0												18%	-7.1	-7.4	-9.1
disodium aniline-2,5-disulphonate	255-250-5	41184-20-7	41184207	5877	Reach_2737	610	297	0.0												18%	-7.1	-7.4	-9.1
O,O-dimethyl hydrogen dithiophosphate	212-053-9	756-80-9	756809	864	Reach_1527	611	158	-82.4	5.5E+01	2.7E+03	1.8E+01	-0.1		2.7E-08	1.1E-07	1.1E-06				22%	-7.7	-7.4	-8.7
2,5-dichlorophenol	209-520-4	583-78-8	583788	728	Reach_1383	612	163	46.8	6.1E+00	3.6E+03	6.3E+02	7.5		1.3E-08	3.5E-08	1.1E-07				23%	-7.7	-7.4	-8.4
2-(2-(2-ethoxyethoxy)ethoxy)ethanol	203-978-9	112-50-5	112505	331	Reach_910	613	178	35.7	3.0E-01	3.8E+06	1.1E-01	14.9		7.0E-07	1.1E-07	3.5E-07				15%	-6.5	-7.4	-9.5
imidazolidine-2-thione	202-506-9	96-45-7	96457	1054	Reach_464	614	102	69.7	2.7E-04	8.1E+05	3.2E-01	13	12	6.3E-09	1.1E-06	3.5E-06				23%	-6.9	-7.4	-8.4
m-phenoxybenzaldehyde	254-487-1	39515-51-0	39515510	625	Reach_2726	615	198	83.6	2.2E-02	4.4E+01	5.9E+03			4.7E-08	1.1E-07	3.5E-07				21%	-7.7	-7.4	-8.7
1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxyli	230-991-7	7397-62-8	7397628	3630	Reach_2247	616	132	-3.1	7.0E+00	2.3E+04	2.4E+00			3.5E-06	3.5E-07	1.1E-06				22%	-7.7	-7.4	-8.7
hex-1-ene	209-753-1	592-41-6	592416	3270	Reach_1392	617	84	-95.3	2.5E+04	1.5E+02	1.4E+03			1.1E-06	1.1E-07	3.5E-07				20%	-7.8	-7.4	-10.4
1,2-benzisothiazol-3(2H)-one 1,1-dioxide, sodium salt	204-886-1	128-44-9	128449	1189	Reach_1111	618	205	0.0												18%	-7.1	-7.4	-9.1
sodium ethanolate	205-487-5	141-52-6	141526	5691	Reach_1163	619	68	0.0												18%	-7.2	-7.4	-9.1
4-isopropylaniline	247-119-6	25586-42-9	25586429	2439	Reach_2570	620	352	167.3	2.9E-06	3.4E-02	1.9E+08			1.1E-06	1.1E-07	3.5E-07				14%	-7.7	-7.4	-9.3
690-526-2	690-526-2	38632-47-2	38632472	5870	Reach_4657	621	376	0.0												18%	-7.1	-7.4	-9.1
1,2,3-trichloropropane	202-486-1	96-18-4	96184	1047	Reach_453	622	147	-46.9	3.9E+02	1.8E+03	3.2E+02			1.5E-08	1.1E-08	3.5E-08				23%	-7.7	-7.4	-9.2
diethyl phthalate	201-550-6	84-66-2	84662	961	Reach_288	623	222	-1.7	3.4E-01	5.3E+02	4.5E+02			8.3E-07	1.1E-07	3.5E-07				15%	-7.7	-7.4	-9.3
triclosan	222-182-2	3380-34-5	3380345	48	Reach_1954	624	290	136.8	6.2E-04	3.0E+00	4.6E+04	8.8		2.2E-09	1.1E-08	3.5E-08				23%	-7.7	-7.4	-8.4
sodium ascorbate	229-352-5	6485-40-1	6485401	781	Reach_2189	625	150	9.9	1.7E+01	1.2E+03	1.2E+03									18%	-7.1	-7.5	-9.1
2,2,2',2'-tetrakis(hydroxymethyl)-3,3'-oxydipropan-1-ol	204-794-1	126-58-9	126589	1808	Reach_1087	626	254	191.9	2.3E-10	1.0E+06	2.5E-03	14.1		1.1E-06	3.5E-07	1.1E-06				14%	-6.4	-7.5	-9.6
1-chloro-2,5-dimethoxy-4-nitrobenzene	230-086-7	6940-53-0	6940530	3543	Reach_2214	627	218	94.9	4.5E-02	9.6E+01	4.2E+02			1.1E-06	1.1E-07	3.5E-07				15%	-7.7	-7.5	-9.3
acetophenone	202-708-7	98-86-2	98862	1077	Reach_521	628	120	-9.9	4.3E+01	3.5E+03	4.7E+01			7.4E-07	3.5E-07	1.1E-06				15%	-7.7	-7.5	-8.9
3-nitrotoluene	221-259-8	3048-64-4	3048644	2599	Reach_1906	629	120	-41.3	1.0E+03	2.7E+02	4.2E+03			1.1E-06	1.1E-07	3.5E-07				23%	-7.7	-7.5	-8.7
hexan-6-olide	207-938-1	502-44-3	502443	2999	Reach_1300	630	114	-21.6	2.3E+01	2.4E+04	4.8E+00			3.5E-06	3.5E-07	1.1E-06				14%	-7.7	-7.5	-9.4
604-340-6	604-340-6	143230-42-6	143230426	1960	Reach_4148	631	353	169.8	1.3E-05	4.1E+01	1.6E+01		13	1.1E-06	1.1E-07	3.5E-07				14%	-6.5	-7.5	-9.5
4,6-dichloro-5-nitro-2-(propylthio)pyrimidine	203-679-3	109-54-6	109546	1502	Reach_776	632	122	-49.8	1.1E+03	8.6E+04	1.9E+01			3.5E-07	3.5E-08	1.1E-07				16%	-7.6	-7.5	-9.3
2,3,5,6-tetrachloropyridine	219-283-9	2402-79-1	2402791	2367	Reach_1796	633	217	54.6	8.1E-01	2.1E+01	2.4E+03			3.5E-08	1.1E-08	3.5E-08				22%	-7.7	-7.5	-8.8
acetylene	200-816-9	74-86-2	74862	3649	Reach_112	634	26	-154.0	2.4E+06	6.2E+03	3.2E+00			1.1E-06	1.1E-07	3.5E-07				20%	-7.9	-7.5	-10.0
1,3,5-triazine-2,4,6-triyltrinitrilohexamethanol	208-503-9	531-18-0	531180	3088	Reach_1328	635	306	243.9	1.1E-12	4.3E+05	3.3E-06	14.7	11.4	1.1E-07	1.1E-07	3.5E-07				19%	-6.5	-7.5	-9.1
tert-butylamine	200-888-1	75-64-9	75649	862	Reach_155	636	73	-64.8	4.7E+04	5.7E+05	5.2E+00		4	8.3E-09	3.5E-07	1.1E-06				23%	-7.8	-7.5	-8.8
tert-butyl [(4R,6R)-6-{2-[2-(4-fluorophenyl)-3-phenyl-4-(phenyl	700-258-0	125971-95-1	125971951	1801	Reach_4827	637	655	347.9	1.7E-17	1.7E-06	3.0E+10	14.3	15.9	3.5E-07	3.5E-08	1.1E-07				16%	-6.9	-7.5	-9.1
629-764-9	629-764-9	164524-02-1	164524021	5732	Reach_4596	638	238	0.0												18%	-7.2	-7.5	-9.1
616-280-8	616-280-8	760108-96-1	760108961	6030	Reach_4429	639	404	0.0												18%	-7.2	-7.5	-9.1
tetramethylammonium hydroxide	200-882-9	75-59-2	75592	6027	Reach_153	640	91	0.0												18%	-7.2	-7.5	-9.1
methylamine	200-820-0	74-89-5	74895	840	Reach_115	641	31	-98.3	3.1E+05	1.0E+06	2.3E-01		3	4.2E-07	3.5E-07	1.1E-06				16%	-8.0	-7.5	-8.7
dodecanedioic acid, compound with hexane-1,6-diamine (1:1)	235-697-2	12542-30-2	12542302	1797	Reach_2314	642	204	44.0	1.0E+00	2.8E+02	1.6E+03									18%	-7.2	-7.5	-9.2
4,4'-methylenedicyclohexyl diisocyanate	225-863-2	5124-30-1	5124301	3030	Reach_2079	643	262	111.7	3.1E-03	1.8E+01	1.3E+06			3.5E-07	3.5E-08	1.1E-07				21%	-7.4	-7.5	-8.9
[(2R*, 4R*) -2-(bromomethyl)-2-(2,4-dichlorophenyl)-1,3-dioxo	222-697-2	3577-63-7	3577637	2748	Reach_1974	644	217	187.2	2.2E-08	1.7E+05	1.6E-02			1.1E-06	1.1E-07	3.5E-07				19%	-6.9	-7.5	-9.1
disodium 4,4'-bis[[4-anilino-6-[(2-carbamoylethyl)(2-hydroxyet	248-420-5	27344-06-5	27344065	5809	Reach_2601	645	1015	0.0												18%	-7.2	-7.5	-9.2
3-nitrobenzaldehyde	210-415-0	615-20-3	615203	3338	Reach_1426	646	170	72.8	4.0E+00	1.5E+02	6.5E+02			3.5E-07	3.5E-08	1.1E-07				20%	-7.8	-7.5	-8.9
2,4-xylidine	611-349-9	560-62-3	560623	3185	Reach_4357	647	302	172.7	2.7E-07	6.8E+01	1.8E+01			3.5E-07	3.5E-08	1.1E-07				16%	-7.7	-7.5	-9.2
α-chlorotoluene	202-853-6	100-44-7	100447	126	Reach_558	648	127	-27.2	1.3E+02	6.6E+02	6.2E+02			8.0E-07	3.5E-08	1.1E-07				16%	-7.8	-7.5	-9.1
methanethiol	200-822-1	74-93-1	74931	3652	Reach_117	649	48	-115.3	2.0E+05	2.3E+04	6.0E+00	10.7		1.1E-07	3.5E-08	3.5E-07				22%	-7.9	-7.5	-9.6
603-525-9	603-525-9	131860-97-4	131860974	1852	Reach_4123	650	321	160.9	2.7E-05	6.3E+01	2.9E+01		12.9	1.1E-06	1.1E-07	3.5E-07				14%	-6.6	-7.5	-9.6
1,4-dichlorobenzene	203-400-5	106-46-7	106467	192	Reach_668	651	147	-14.3	8.8E+01	1.2E+02	1.9E+03			2.3E-09	1.1E-08	3.5E-08				24%	-7.8	-7.5	-9.4
androst-4-ene-3,17-dione	200-554-5	63-05-8	63058	75	Reach_67	652	286	145.2	2.4E-04	2.2E+01	5.8E+02			3.3E-07	3.5E-08	1.1E-07				16%	-7.4	-7.5	-9.3

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
5-amino-1,3-dihydro-2H-benzimidazol-2-one	202-401-8	95-23-8	95238	4123	Reach_424	653	149	130.5	1.6E-03	9.4E+03	1.9E+00	13	7.99	3.5E-07	3.5E-08	3.5E-07				16%	-6.6	-7.5	-9.4
4-nitrotoluene-2-sulphonic acid	204-445-3	121-03-9	121039	1722	Reach_1007	654	217	150.6	2.9E-06	7.9E+02	1.6E-01	0.18		3.5E-06	3.5E-08	1.1E-07				14%	-6.4	-7.5	-9.9
4-nitrobenzoic acid	200-526-2	62-23-7	62237	761	Reach_62	655	167	115.9	3.4E-04	3.8E+02	4.9E+01	3.3		2.3E-07	1.1E-07	3.5E-07				17%	-6.9	-7.5	-9.3
cyclohexane-1,2-dicarboxylic anhydride	201-604-9	85-42-7	85427	3889	Reach_295	656	154	-1.8	7.1E+00	3.7E+03	1.5E+02			1.1E-06	3.5E-07	1.1E-06				15%	-7.8	-7.5	-9.3
aluminium trilactate	242-670-9	18917-91-4	18917914	5751	Reach_2471	657	294	0.0												18%	-7.2	-7.5	-9.2
tetramethylthiuram monosulphide	202-605-7	97-74-5	97745	1059	Reach_486	658	208	88.5	3.6E-02	1.9E+03	5.6E+00			2.5E-08	1.1E-07	3.5E-07				22%	-7.6	-7.5	-8.7
caffeine	202-078-3	91-57-6	91576	1007	Reach_376	659	142	22.2	4.6E+00	1.0E+01	5.2E+03			4.5E-08	3.5E-08	1.1E-07				23%	-6.8	-7.5	-8.5
ziram (reach)	205-288-3	137-30-4	137304	6353	Pest_436	660														18%	-7.2	-7.5	-9.2
fluorouracil	228-761-6	6358-08-3	6358083	1283	Reach_2166	661	189	127.8	8.9E-04	5.0E+02	4.4E+01	6.32		3.5E-06	1.1E-07	3.5E-07				17%	-6.6	-7.5	-9.3
flumetasone	639-824-6	1229457-94-6	1229457946	1759	Reach_4607	662	277	114.9	9.5E-03	1.3E+04	1.1E+02			1.1E-05	3.5E-07	1.1E-06				19%	-7.0	-7.5	-9.1
1,2,3,6-tetrahydrophthalic anhydride	201-605-4	85-43-8	85438	3890	Reach_296	663	152	-0.7	7.7E+00	1.0E+04	9.1E+01			3.5E-06	3.5E-07	3.5E-07				14%	-7.8	-7.5	-9.5
acetaldehyde	200-836-8	75-07-0	75070	848	Reach_127	664	44	-106.4	1.2E+05	5.7E+05	6.8E-01			4.5E-06	1.1E-06	3.5E-06				14%	-7.8	-7.5	-9.1
octadecyl methacrylate	251-013-5	32360-05-7	32360057	2649	Reach_2660	665	339	99.6	6.4E-04	1.3E-04	4.2E+09			1.1E-06	1.1E-07	3.5E-07				23%	-7.5	-7.6	-8.8
malononitrile	203-703-2	109-77-3	109773	266	Reach_791	666	66	-12.3	1.5E+01	6.9E+04	2.5E-01			4.0E-07	1.1E-07	3.5E-07				16%	-7.7	-7.6	-9.4
strontium 4-[(5-chloro-4-methyl-2-sulphonatophenyl)azo]-3-hy	239-879-2	15782-05-5	15782055	5724	Reach_2397	667	506	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.2	-7.6	-9.2
hexane-1,6-diaminium benzene-1,4-dicarboxylate	700-230-8	3160-86-9	3160869	5840	Reach_4813	668	282	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.2	-7.6	-9.2
688-329-1	688-329-1	10175-31-2	10175312	1327	Reach_4643	669	170	17.6	1.6E+01	1.3E+03	2.5E+02		5.76	3.5E-07	3.5E-08	1.1E-07				16%	-7.8	-7.6	-8.9
N-methyldidecylamine	230-990-1	7396-58-9	7396589	3629	Reach_2246	670	312	90.4	2.8E-03	3.2E-04	7.6E+08		3.6	1.1E-06	1.1E-07	3.5E-07				23%	-7.4	-7.6	-9.1
trimethyl borate	204-468-9	121-43-7	121437	1726	Reach_1012	671	104	-82.6	2.0E+04		1.3E-02			1.1E-06	3.5E-07	1.1E-06				14%	-7.7	-7.6	-9.6
sodium hydrogen-5-sulphoisophthalate	228-845-2	6362-79-4	6362794	5962	Reach_2173	672	268	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.2
disulfiram	202-607-8	97-77-8	97778	1060	Reach_487	673	297	138.9	8.8E-04	9.7E+00	4.7E+03		16	2.7E-08	3.5E-07	1.1E-06				22%	-7.4	-7.6	-8.8
potassium sodium 4,4'-bis[6-anilino-4-[bis(2-hydroxyethyl)amir	275-031-8	70942-01-7	70942017	6007	Reach_2923	674	977	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.2	-7.6	-9.2
benzyltrimethylammonium chloride	200-300-3	56-93-9	56939	1222	Reach_34	675	186	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.2
3,6,9,12-tetraoxotridecanol	245-883-5	23783-42-8	23783428	2359	Reach_2535	676	208	62.1	1.4E-02	2.0E+05	1.9E-02	14.9		1.1E-06	3.5E-07	3.5E-07				14%	-6.6	-7.6	-9.7
methylphosphonic acid, compound with amidinourea (1:1)	282-758-4	84402-58-4	84402584	6051	Reach_2972	677	198	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.2
trimethylamine	200-875-0	75-50-3	75503	859	Reach_147	678	59	-109.9	2.2E+05	4.2E+05	1.1E+00		4	5.5E-07	1.1E-07	3.5E-07				16%	-8.0	-7.6	-9.1
sodium hydrogen [N,N-bis[2-[bis(carboxymethyl)amino]ethyl]g	235-627-0	12389-75-2	12389752	5635	Reach_2313	679	468	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.2
biphenyl-2-ol	201-993-5	90-43-7	90437	106	Reach_364	680	170	86.6	9.4E-02	2.5E+02	1.9E+03	10		5.7E-07	3.5E-08	3.5E-08				16%	-7.8	-7.6	-9.4
cholic acid	201-337-8	81-25-4	81254	100	Reach_274	681	409	233.4	1.3E-12	1.1E+02	3.3E+03	4.89		3.1E-07	1.1E-07	3.5E-07				16%	-7.1	-7.6	-9.3
chlorobenzene	203-628-5	108-90-7	108907	248	Reach_761	682	113	-45.8	1.2E+03	2.0E+02	4.4E+02			2.2E-09	1.1E-08	3.5E-08				24%	-8.0	-7.6	-10.0
601-639-3	218-817-8	2243-62-1	2243621	542	Reach_1779	683	158	109.7	5.0E-04	1.2E+03	2.2E+01			2.6E-09	1.1E-07	1.1E-06				17%	-7.8	-7.6	-9.4
sulfapyridine	205-642-7	144-83-2	144832	29	Reach_1196	684	249	176.4	5.5E-06	2.5E+03	3.4E+00	8.78	11	4.3E-09	1.1E-07	1.1E-06				23%	-7.1	-7.6	-8.5
isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-dio	246-771-9	25265-77-4	25265774	2426	Reach_2563	685	216	24.8	6.4E-01	1.1E+03	1.0E+03	15.4		3.5E-06	3.5E-07	1.1E-06				14%	-7.8	-7.6	-9.5
triisobutyl phosphate	204-798-3	126-71-6	126716	18	Reach_1088	686	266	16.4	1.7E+00	3.1E+02	4.0E+03			2.6E-08	1.1E-07	3.5E-07				22%	-7.9	-7.6	-8.8
2-(ethylthio)ethanol	203-802-0	110-77-0	110770	283	Reach_828	687	106	-26.6	2.5E+01	1.5E+04	2.8E+00	15		3.0E-08	1.1E-06	3.5E-06				22%	-7.9	-7.6	-8.8
guanidinium phosphate (1:1)	226-551-9	5423-22-3	5423223	5924	Reach_2110	688	157	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.2
morpholinium toluene-4-sulphonate	237-301-3	13732-62-2	13732622	5681	Reach_2346	689	259	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.2
2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2-me	226-789-3	5468-75-7	5468757	3152	Reach_2118	690	658	349.8	2.7E-20	1.4E-05	1.0E+07	8.45	13.4	3.5E-07	3.5E-08	3.5E-08				16%	-7.3	-7.6	-9.5
hexasodium 2,2'-[vinylenebis[(3-sulphonato-4,1-phenylene)imi	255-217-5	41098-56-0	41098560	5875	Reach_2735	691	1305	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.3
2-ethylhexyl palmitate	249-862-1	29806-73-3	29806733	2572	Reach_2631	692	369	117.2	1.4E-04	3.9E-05	4.1E+10			1.1E-06	1.1E-07	3.5E-07				24%	-7.7	-7.6	-8.5
3,7,11,15-tetramethylhexadec-1-en-3-ol	208-008-8	505-32-8	505328	3007	Reach_1307	693	297	70.2	1.9E-03	8.1E-02	1.7E+08	15.5		3.5E-07	3.5E-08	1.1E-07				23%	-7.4	-7.6	-8.5
2,6-diisopropylaniline	246-305-4	24544-04-5	24544045	560	Reach_2548	694	177	51.0	2.5E+00	1.3E+01	9.8E+03		10	6.3E-09	3.5E-08	1.1E-07				23%	-7.9	-7.6	-8.6
2-methyl-p-phenylenediamine sulfate	210-431-8	615-50-9	615509	5951	Reach_1427	695	220	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.2
sodium calcium edetate	200-529-9	62-33-9	62339	5957	Reach_63	696	374	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.3
tris(2-hydroxyethyl)-1,3,5-triazinetrione	212-660-9	839-90-7	839907	3854	Reach_1564	697	261	240.8	1.2E-13	7.6E+05	1.2E+00	14.9	14.6	3.5E-06	1.1E-06	3.5E-06				14%	-6.5	-7.6	-9.5
calcium bis[4-[[1-[[(2-methylphenyl)amino]carbonyl]-2-oxoprop	235-558-6	12286-66-7	12286667	5632	Reach_2312	698	879	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.3
linalool	201-134-4	78-70-6	78706	899	Reach_205	699	154	-11.4	1.1E+01	8.0E+02	2.4E+03	15.5		3.2E-07	1.1E-07	3.5E-07				17%	-7.9	-7.6	-8.9
2-phenyl-1H-benzimidazole-5-sulphonic acid	248-502-0	27503-81-7	27503817	42	Reach_2608	700	274	243.5	9.8E-13	1.2E+03	6.9E-01	-0.41	9.03	2.2E-09	3.5E-08	3.5E-08				23%	-6.8	-7.6	-8.5
sodium 1,4-diisodecyl sulphonatosuccinate	249-894-6	29857-13-4	29857134	5826	Reach_2633	701	501	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.3
fumaric acid	203-743-0	110-17-8	110178	276	Reach_807	702	116	84.1	1.3E-09	5.5E+04	1.1E+00	3		4.7E-06	3.5E-07	1.1E-06				14%	-6.4	-7.6	-9.6
sodium salicylate	200-198-0	54-21-7	54217	1219	Reach_22	703	160	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.3
norflurane	212-377-0	811-97-2	811972	3803	Reach_1549	704	102	-150.5	5.3E+05	3.2E+03	4.8E+01			3.5E-08	1.1E-08	3.5E-08				23%	-8.1	-7.6	-10.3
prednisolone	200-021-7	50-24-8	50248	656	Reach_6	705	360	215.3	9.1E-12	4.4E+02	2.5E+01	13.2		1.4E-07	3.5E-07	1.1E-06				18%	-7.0	-7.6	-9.2
m-cresol	203-577-9	108-39-4	108394	237	Reach_743	706	108	15.7	2.2E+01	1.6E+04	1.1E+02	10		2.8E-06	1.1E-06	3.5E-06				14%	-7.9	-7.6	-9.5
hesperidin	208-288-1	520-26-3	520263	3051	Reach_1322	707	611	349.8	1.6E-24	1.7E+03	1.9E-01	9.26		1.1E-06	1.1E-07	3.5E-07				14%	-6.5	-7.6	-9.8
(±)-2-(6-methoxy-2-naphthyl)propionic acid	247-485-7	26159-31-9	26159319	572	Reach_2575	708	230	137.6	1.7E-04	2.8E+02	1.3E+03	4.36		8.0E-09	1.1E-07	3.5E-07				23%	-7.4	-7.6	-8.6
N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxobutyramide	247-820-7	26576-46-5	26576465	2478	Reach_2588	709	233	199.5	2.7E-07	1.3E+04	1.7E+00	10.6	11.7	3.5E-07	3.5E-08	1.1E-07				16%	-6.5	-7.6	-9.5
dimethyl disulphide	210-871-0	624-92-0	624920	764	Reach_1456	710	94	-69.7	3.3E+03	5.1E+03	7.4E+01			2.2E-09	3.5E-08	3.5E-07				24%	-7.9	-7.6	-9.4
sodium 2-methylprop-2-ene-1-sulphonate	216-341-5	1561-92-8	1561928	5718	Reach_1691	711	158	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.3
potassium O-pentyl dithiocarbonate	220-329-5	2720-73-2	2720732	1211	Reach_1858	712	202	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.3
dipotassium adipate	242-838-1	19147-16-1	19147161	5754	Reach_2474	713	222	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.3
2,2-bis(chloromethyl)trimethylene bis(bis(2-chloroethyl)phospl	253-760-2	38051-10-4	38051104	2812	Reach_2714	714	583	90.3	2.7E-06	2.4E-01	2.0E+03			3.5E-07	3.5E-08	1.1E-07				17%	-7.6	-7.6	-9.4
oxalic acid	205-634-3	144-62-7	144627	472	Reach_1195	715	90	63.0	7.5E-01	7.3E+05	1.8E-02	1.2		4.7E-06	3.5E-07	1.1E-06				14%	-6.4	-7.6	-9.7
acrylaldehyde	203-453-4	107-02-8	107028	205	Reach_690	716	56	-94.6	3.5E+04	2.5E+05	1.5E+00			4.5E-06	1.1E-06	3.5E-06				14%	-7.9	-7.6	-9.2
carbonic acid, compound with 2-aminoethanol (1:2)	244-600-2	21829-52-7	21829527	5775	Reach_2510	717	184	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.3
2,4-dinitrophenol	200-087-7	51-28-5	51285	57	Reach_14	718	184	118.5	1.7E-03	2.1E+03	5.4E+01	4.2		2.2E-09	3.5E-08	1.1E-07				23%	-7.1	-7.6	-8.6
D-gluconic acid	208-401-4	526-95-4	526954	3069	Reach_1324	719	196	161.7	1.1E-07	7.2E+05	1.3E-02	3.36		3.5E-06	3.5E-07	1.1E-06				14%	-6.3	-7.6	-9.7
calcium(2+) 12-hydroxyoctadecanoate	221-605-8	3159-62-4	3159624	5839	Reach_1922	720	639	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.3
trichloroacetic acid	200-927-2	76-03-9	76039	90	Reach_170	721	163	26.7	2.6E+01	1.6E+05	2.8E+01	0.6		5.8E-08	1.1E-07	3.5E-07				20%	-7.1	-7.6	-9.0
xylose	200-400-7	58-86-6	58866	3256	Reach_49	722	150	96.3	1.0E-04	1.0E+06	1.0E-02	12.5		3.5E-06	1.1E-06	3.5E-06				14%	-6.6	-7.6	-9.7
1-(7-bromo-9,9-difluoro-9H-fluoren-2-yl)-2-chloroethanone	203-483-8	107-35-7	107357	1460	Reach_705	723	125	70.9	2.3E-05	2.1E+05	4.4E-04	-0.3	5	3.5E-06	1.1E-06	3.5E-06				16%	-6.6	-7.6	-9.6
terephthaloyl dichloride	202-829-5	100-20-9	100209	1297	Reach_551	724	203	68.2	6.5E-01	7.1E+02	7.6E+00			3.5E-06	3.5E-07	1.1E-06				14%	-7.9	-7.6	-9.6
diammonium [N,N-bis[2-[bis(carboxymethyl)amino]ethyl]glycir	289-064-0	85959-68-8	85959688	6062	Reach_2988	725	480	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.6	-9.3
triphenyl phosphate	233-713-2	10326-41-7	10326417	161	Reach_2288	726	90	22.7	3.8E+00	7.7E+05	2.2E-01			4.7E-07	3.5E-07	3.5E-07				17%	-7.7	-7.6	-9.4
dimethyl ether	204-065-8	115-10-6	115106	1630	Reach_936	727	46	-128.1	5.1E+05	2.0E+05	1.2E+00			1.1E-06	1.1E-07	3.5E-07				16%	-8.1	-7.6	-9.3

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
(3-chloropropyl)triethoxysilane	225-805-6	5089-70-3	5089703	3022	Reach_2077	728	241	29.4	2.3E+00	1.8E+02	1.1E+02			3.5E-07	1.1E-07	3.5E-07				16%	-7.9	-7.6	-9.0
aspartic acid	200-291-6	56-84-8	56848	3212	Reach_31	729	133	218.2	3.5E-05	1.9E+05	4.8E-05	1.7	4.1	3.5E-06	3.5E-07	1.1E-06				14%	-6.4	-7.6	-9.7
n-hexane	203-777-6	110-54-3	110543	279	Reach_817	730	86	-93.8	2.0E+04	9.1E+01	1.9E+03			1.6E-06	3.5E-08	1.1E-07				20%	-8.0	-7.6	-10.7
4-(2-hydroxypropan-2-yl)-2-propyl-1-{[2'-(1H-tetrazol-5-yl)biph	209-057-8	554-00-7	554007	700	Reach_1362	731	162	46.2	2.0E+00	1.8E+02	2.3E+02		12	2.2E-09	1.1E-08	3.5E-08				16%	-7.0	-7.6	-9.6
sodium hydrogen [6R-(6α,7β)]-3-(acetoxymethyl)-7-[(5-amino-	203-227-5	104-68-7	104687	1399	Reach_627	732	182	59.4	1.3E-02	1.7E+04	6.8E+00									18%	-7.3	-7.6	-9.3
triethylamine	204-469-4	121-44-8	121448	370	Reach_1013	733	101	-70.6	7.9E+03	4.8E+04	3.2E+01		3	1.5E-08	3.5E-07	1.1E-06				23%	-7.9	-7.6	-9.2
2-ethylhexanal	204-596-5	123-05-7	123057	1761	Reach_1038	734	128	-42.3	2.9E+02	4.4E+02	5.1E+02			3.5E-07	1.1E-07	3.5E-07				18%	-7.9	-7.6	-9.5
6H-dibenz[c,e][1,2]oxaphosphorin 6-oxide	252-813-7	35948-25-5	35948255	2754	Reach_2696	735	216	84.0	3.8E-03	1.9E+02	7.4E+01			3.5E-07	3.5E-08	3.5E-08				16%	-7.5	-7.6	-9.5
pyrocatechol	204-427-5	120-80-9	120809	361	Reach_1002	736	110	45.7	1.5E-01	8.8E+04	1.1E+01	10		4.1E-06	3.5E-07	1.1E-06				14%	-6.9	-7.6	-9.6
4-chlorobenzenesulphonyl chloride	200-870-3	75-44-5	75445	3672	Reach_144	737	99	-67.5	1.8E+05	9.7E+03	1.9E-01			1.1E-07	3.5E-08	3.5E-08				19%	-7.9	-7.6	-9.2
2'-methoxyacetoacetanilide	202-131-0	92-15-9	92159	4029	Reach_383	738	207	137.5	1.2E-03	5.7E+03	3.4E+00	10.7	13.7	1.1E-06	1.1E-07	3.5E-07				14%	-6.7	-7.6	-9.7
3-methylbut-3-en-1-ol	212-110-8	763-32-6	763326	3709	Reach_1536	739	86	-60.1	4.9E+02	9.6E+03	1.8E+01	15.9		3.5E-06	1.1E-06	3.5E-06				14%	-7.9	-7.6	-9.2
[(butoxymethylethoxy)methylethoxy]propan-1-ol	259-910-3	55934-93-5	55934935	3182	Reach_2811	740	248	54.6	7.7E-03	6.2E+02	1.9E+01	13.5		1.1E-06	3.5E-07	1.1E-06				14%	-7.5	-7.7	-9.6
proxan-sodium	205-443-5	140-93-2	140932	1197	Reach_1154	741	158	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.7	-9.3
(E)-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	201-224-3	79-77-6	79776	926	Reach_249	742	192	52.5	3.0E+00	3.2E+02	2.6E+04			6.3E-08	3.5E-07	1.1E-06				21%	-7.9	-7.7	-8.9
2-chloropropionic acid	209-952-3	598-78-7	598787	3293	Reach_1406	743	109	8.1	1.0E+02	1.6E+05	5.8E+00	2.9		1.1E-06	1.1E-07	3.5E-07				14%	-6.6	-7.7	-9.7
4,4'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[2,4-dihy	239-898-6	15793-73-4	15793734	2057	Reach_2399	744	652	349.8	2.3E-19	1.1E-05	1.8E+11		13.3	3.5E-07	3.5E-08	3.5E-08				16%	-7.1	-7.7	-9.0
perylene-3,4:9,10-tetracarboxydiimide	201-344-6	81-33-4	81334	3804	Reach_275	745	390	349.8	4.4E-21	1.8E-02	5.8E+03	9.3	12.8	1.1E-07	3.5E-09	1.1E-08				19%	-7.0	-7.7	-9.3
dichlobenil (reach)	214-787-5	1194-65-6	1194656	352	Reach_1672	746	172	52.7	7.8E-02	6.3E+01	6.8E+02			3.2E-09	1.1E-08	3.5E-08				23%	-7.9	-7.7	-8.7
N,N-diethylaniline	202-088-8	91-66-7	91667	1009	Reach_378	747	149	-1.4	2.1E+01	1.6E+03	1.4E+03		8	1.7E-08	1.1E-07	3.5E-07				22%	-7.9	-7.7	-8.6
tetrakis(hydroxymethyl)phosphonium sulphate(2:1)	259-709-0	55566-30-8	55566308	1221	Reach_2809	748	406	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.7	-9.3
4-(2-aminoethyl)benzenesulphonamide	252-501-0	35303-76-5	35303765	2729	Reach_2688	749	200	126.6	1.4E-03	1.8E+03	5.2E-01	10.3	4.98	3.5E-07	3.5E-08	1.1E-07				16%	-6.8	-7.7	-9.6
sodium diisobutylnaphthalenesulphonate	248-326-4	27213-90-7	27213907	5808	Reach_2598	750	342	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.3	-7.7	-9.3
trichloro(3-chloropropyl)silane	219-844-8	2550-06-3	2550063	1251	Reach_1837	751	212	-18.8	1.2E+02	3.8E+03	1.7E+03			1.1E-07	1.1E-08	3.5E-08				19%	-7.9	-7.7	-9.0
octan-1-ol	203-917-6	111-87-5	111875	314	Reach_878	752	130	-14.5	1.3E+01	6.2E+02	6.5E+02	15.9		3.8E-06	3.5E-07	1.1E-06				14%	-7.9	-7.7	-9.3
8,18-dichloro-5,15-diethyl-5,15-dihydrodiindolo[3,2-b:3',2'-m]t	228-767-9	6358-30-1	6358301	3406	Reach_2167	753	589	339.3	7.1E-17	1.6E-05	2.1E+09			3.5E-07	1.1E-08	3.5E-08				23%	-7.7	-7.7	-8.3
mycophenolic acid	246-119-3	24280-93-1	24280931	2383	Reach_2541	754	320	215.6	2.1E-08	2.7E+02	1.7E+04	4.89		1.1E-06	1.1E-07	3.5E-07				14%	-7.0	-7.7	-9.6
nitrilotriacetonitrile	230-804-9	7327-60-8	7327608	3617	Reach_2237	755	134	92.8	8.2E-03	8.9E+05	4.1E-02			3.5E-07	1.1E-07	3.5E-07				16%	-6.7	-7.7	-9.6
hydrocortisone	200-020-1	50-23-7	50237	655	Reach_5	756	362	214.5	1.6E-11	4.7E+02	4.2E+01	13.2		2.1E-07	1.1E-07	3.5E-07				17%	-6.9	-7.7	-9.4
o-(p-isocyanatobenzyl)phenyl isocyanate	227-534-9	5873-54-1	5873541	3254	Reach_2139	757	250	98.7	6.3E-03	3.5E+01	1.7E+05			1.1E-06	1.1E-07	3.5E-07				18%	-7.8	-7.7	-9.4
hexadec-1-ene	211-105-8	629-73-2	629732	3391	Reach_1470	758	224	21.3	1.0E+00	8.1E-03	1.1E+08			1.1E-06	1.1E-07	3.5E-07				23%	-7.6	-7.7	-9.8
quinoline	202-051-6	91-22-5	91225	1006	Reach_374	759	129	37.6	7.2E+00	3.5E+02	1.4E+02		9	9.5E-08	1.1E-07	3.5E-07				19%	-7.9	-7.7	-9.1
3-(difluoromethyl)-1-methyl-1H-pyrazole-4-carboxylic acid	204-004-5	112-76-5	112765	1602	Reach_923	760	303	95.4	3.4E-02	4.8E-04	2.5E+07			1.1E-06	1.1E-07	3.5E-07				14%	-6.7	-7.7	-9.7
cyclohexylamine	203-629-0	108-91-8	108918	249	Reach_762	761	99	-27.1	1.1E+03	9.1E+03	4.3E+01		4	3.2E-07	3.5E-07	1.1E-06				17%	-8.0	-7.7	-9.1
2,6-di-tert-butyl-p-cresol	204-881-4	128-37-0	128370	413	Reach_1108	762	220	83.0	2.4E-01	1.6E+00	1.1E+05	12.1		2.4E-09	3.5E-07	1.1E-06				24%	-7.9	-7.7	-9.2
cetrimonium chloride	203-928-6	112-02-7	112027	7	Reach_884	763	320	212.6	3.7E-08	5.9E-03	1.5E+03			4.6E-07	1.1E-07	3.5E-07				16%	-7.4	-7.7	-9.5
611-255-8	629-377-5	67442-07-3	67442073	3491	Reach_4592	764	138	20.3	2.2E+01	9.3E+04	2.1E+00			3.5E-07	3.5E-08	1.1E-07				16%	-7.1	-7.7	-9.6
acetonitrile	200-835-2	75-05-8	75058	847	Reach_126	765	41	-83.8	2.7E+04	1.8E+05	7.1E-01			8.3E-07	1.1E-07	3.5E-07				15%	-8.0	-7.7	-9.0
6-methyl-1,2,3-oxathiazin-4(3H)-one 2,2-dioxide, potassium sal	259-715-3	55589-62-3	55589623	63	Reach_2810	766	201	224.7	5.8E-09		5.0E-03	8.22		8.2E-07	1.1E-06	3.5E-06				15%	-6.7	-7.7	-9.6
3,5,5-trimethylhexanoic acid	221-975-0	3302-10-1	3302101	1259	Reach_1944	767	158	37.4	6.1E+00	4.9E+01	2.2E+03	4.9		3.5E-06	3.5E-07	1.1E-06				14%	-7.9	-7.7	-9.6
propan-1-ol	200-746-9	71-23-8	71238	817	Reach_99	768	60	-75.0	3.1E+03	1.7E+05	2.2E+00	15.9		4.3E-06	1.1E-06	3.5E-06				14%	-7.9	-7.7	-9.3
tetrabutylammonium bromide	216-699-2	1643-19-2	1643192	1201	Reach_1703	769	322	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.4	-7.7	-9.3
azelaic acid	204-669-1	123-99-9	123999	1782	Reach_1064	770	188	127.2	3.1E-03	3.8E+03	5.0E+01	4.59		1.1E-06	3.5E-07	1.1E-06				14%	-7.0	-7.7	-9.6
3-aminopropyltriethoxysilane	213-048-4	919-30-2	919302	4023	Reach_1589	771	221	55.9	9.8E+00	2.8E+04	2.0E+00		4.07	1.1E-06	3.5E-07	1.1E-06				14%	-7.9	-7.7	-9.6
dibenzoyl peroxide	202-327-6	94-36-0	94360	4103	Reach_414	772	242	-2.1	9.3E-03	1.4E+02	2.7E+03			1.1E-06	1.1E-07	3.5E-07				15%	-7.9	-7.7	-9.6
tetrachlorophthalic anhydride	204-171-4	117-08-8	117088	1655	Reach_957	773	286	111.1	6.9E-05	6.6E+00	4.5E+04			1.1E-07	3.5E-08	1.1E-07				20%	-7.6	-7.7	-9.2
α,2-dichlorotoluene	226-009-1	5216-25-1	5216251	3054	Reach_2086	774	230	40.5	3.3E+00	3.6E+00	3.5E+04			1.1E-07	1.1E-08	3.5E-08				21%	-8.0	-7.7	-9.5
3,3',3'',5,5',5''-hexa-tert-butyl-α,α',α''-(mesitylene-2,4,6-triyl)tri	216-971-0	1709-70-2	1709702	2121	Reach_1711	775	775	349.8	4.2E-20	3.7E-14	1.5E+17	10.8		1.1E-06	3.5E-08	1.1E-07				24%	-7.9	-7.7	-6.0
icosan-1-ol	211-119-4	629-96-9	629969	3393	Reach_1472	776	299	104.9	6.7E-05	9.4E-04	5.0E+08	15.9		1.1E-06	3.5E-07	1.1E-06				23%	-7.4	-7.7	-8.6
1,3-bis(hydroxymethyl)-5,5-dimethylimidazolidine-2,4-dione	229-222-8	6440-58-0	6440580	779	Reach_2186	777	188	171.3	1.4E-07	4.6E+05	4.3E-03	14.2	15	1.6E-07	3.5E-07	1.1E-06				18%	-6.7	-7.7	-9.3
m-phenylenediamine	203-584-7	108-45-2	108452	1484	Reach_746	778	108	52.8	2.5E-01	2.0E+04	4.1E-01		8.9	1.1E-06	1.1E-07	1.1E-06				14%	-6.7	-7.7	-9.7
2-diphenylphosphinobenzoic acid	623-635-0	27298-98-2	27298982	2498	Reach_4577	779	135	17.6	2.7E+01	1.5E+03	1.1E+02			3.5E-07	3.5E-08	1.1E-07				16%	-7.3	-7.7	-9.6
ephedrine hydrochloride	200-908-9	75-85-4	75854	865	Reach_164	780	88	-61.0	2.4E+03	1.1E+05	1.7E+01									18%	-7.4	-7.7	-9.4
sodium 2-[(2-aminoethyl)amino]ethanesulphonate	201-940-6	89-79-2	89792	995	Reach_352	781	154	-4.9	6.6E-01	1.4E+03	2.3E+03									18%	-7.4	-7.7	-9.4
sodium 5-oxo-L-prolinate	202-848-9	100-40-3	100403	1305	Reach_555	782	108	-61.9	1.8E+03	5.9E+01	5.4E+03									18%	-7.4	-7.7	-9.4
magnesium acrylate	227-177-9	5698-98-6	5698986	5937	Reach_2132	783	166	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.4	-7.7	-9.4
618-804-0	618-804-0	919-94-8	919948	4026	Reach_4500	784	116	-68.4	5.3E+03	5.2E+03	2.6E+02			1.1E-06	1.1E-07	3.5E-07				16%	-8.0	-7.7	-9.8
perhydro-1,3,5-trinitro-1,3,5-triazine	204-500-1	121-82-4	121824	375	Reach_1019	785	222	132.8	1.8E-04	1.0E+06	4.8E+00			3.9E-07	3.5E-08	1.1E-07				16%	-6.7	-7.7	-9.7
diphenyl ether	202-981-2	101-84-8	101848	150	Reach_584	786	170	35.4	2.3E+00	3.8E+01	1.1E+04			5.0E-09	1.1E-07	3.5E-07				23%	-8.0	-7.7	-9.1
2-chlorobenzamide	210-536-9	617-89-0	617890	3353	Reach_1436	787	97	-8.1	6.6E+02	1.1E+05	2.8E+00			1.1E-06	3.5E-07	1.1E-06				16%	-7.5	-7.7	-9.6
601-672-3	601-672-3	120118-14-1	120118141	1705	Reach_4099	788	218	168.1	4.3E-06	3.8E+01	1.3E+03	7.88	15.6	3.5E-07	3.5E-08	1.1E-07				16%	-7.1	-7.7	-9.6
benzaldehyde	202-860-4	100-52-7	100527	130	Reach_562	789	106	-22.0	1.3E+02	4.9E+03	5.1E+01			1.1E-06	3.5E-07	1.1E-06				15%	-8.0	-7.7	-9.1
isobutyrophenone	227-824-5	5994-61-6	5994616	3297	Reach_2149	790	227	304.0	2.6E-11	1.1E+04	1.3E-05			3.5E-07	1.1E-07	3.5E-07				16%	-8.0	-7.7	-9.0
2-chlorobuta-1,3-diene	204-818-0	126-99-8	126998	1810	Reach_1094	791	89	-105.8	2.9E+04	2.2E+03	3.4E+02			1.1E-06	1.1E-07	3.5E-07				19%	-8.0	-7.7	-10.4
3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H	231-710-0	7695-91-2	7695912	3727	Reach_2270	792	473	203.0	5.4E-06	1.8E-06	1.8E+12			1.1E-06	1.1E-07	3.5E-07				24%	-7.9	-7.7	-8.2
4-(chloromethyl)-5-methyl-1,3-dioxol-2-one	251-203-8	32768-54-0	32768540	2661	Reach_2666	793	161	3.6	3.3E+01	6.1E+01	6.8E+03			1.1E-07	1.1E-08	3.5E-08				16%	-7.1	-7.7	-9.6
choline hydroxide	204-625-1	123-41-1	123411	5634	Reach_1049	794	121	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.4	-7.7	-9.4
sodium mercaptoacetate	206-696-4	367-51-1	367511	5861	Reach_1254	795	114	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.4	-7.7	-9.4
2,4-di-tert-butylphenol	202-532-0	96-76-4	96764	4153	Reach_470	796	206	77.0	3.6E-01	1.3E+01	2.1E+05	10.8		3.5E-06	3.5E-07	1.1E-06				18%	-7.9	-7.7	-9.4
tetrachloro-p-benzoquinone	204-274-4	118-75-2	118752	1677	Reach_969	797	246	102.1	3.0E-04	6.3E+02	1.7E+02			1.1E-07	1.1E-08	3.5E-08				19%	-7.0	-7.7	-9.3
1,1-dichloroethylene	200-864-0	75-35-4	75354	857	Reach_140	798	97	-104.4	8.0E+04	3.5E+03	1.3E+02			1.9E-08	3.5E-08	1.1E-07				24%	-8.1	-7.7	-10.3
5,12-dihydro-2,9-dimethylquino[2,3-b]acridine-7,14-dione	213-561-3	980-26-7	980267	4177	Reach_1624	799	340	247.1	1.9E-12	3.3E-02	6.0E+04	10.8	14	3.5E-07	1.1E-08	3.5E-08				18%	-7.0	-7.7	-9.4
L-alanine	200-273-8	56-41-7	56417	3198	Reach_28	800	89	244.1	3.6E-06	5.6E+05	1.0E-03	2.3	4.2	1.1E-06	3.5E-07	3.5E-07				14%	-6.5	-7.7	-9.8
butyl methacrylate	202-615-1	97-88-1	97881	1061	Reach_490	801	142	-42.7	3.3E+02	1.3E+03	5.6E+02			7.5E-07	3.5E-07	1.1E-06				16%	-8.0	-7.7	-9.4
1,1',1'',1'''-ethylenedinitrilotetrapropan-2-ol	203-041-4	102-60-3	102603	1347	Reach_594	802	292	153.5	1.2E-06	3.1E+05	8.3E-03	14.3	6.78	1.1E-06	3.5E-07	1.1E-06				14%	-6.6	-7.7	-9.8

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
2-chlorobenzonitrile	212-836-5	873-32-5	873325	3927	Reach_1581	803	138	22.9	5.7E+00	2.3E+03	1.5E+02			1.1E-07	1.1E-08	3.5E-08				19%	-8.0	-7.7	-9.1
L-xylo-hex-2-ulosonic acid	208-403-5	526-98-7	526987	3071	Reach_1325	804	194	157.8	8.1E-08	2.0E+05	8.9E-04	1.59		3.5E-06	3.5E-07	1.1E-06				14%	-6.4	-7.7	-9.8
sodium O,O-diisobutyl dithiophosphate	258-508-5	53378-51-1	53378511	5920	Reach_2792	805	264	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.4	-7.7	-9.4
4-(α,α-dimethylbenzyl)phenol	209-968-0	599-64-4	599644	3299	Reach_1410	806	212	102.7	3.9E-03	1.3E+01	1.3E+04	10		3.5E-07	1.1E-07	3.5E-07				17%	-7.9	-7.7	-9.4
612-366-4	612-366-4	6172-80-1	6172801	3350	Reach_4375	807	136	-33.3	1.7E+02	3.2E+04	2.3E+00			1.1E-06	3.5E-07	1.1E-06				14%	-8.0	-7.7	-9.4
ethylene di(acetate)	203-881-1	111-55-7	111557	305	Reach_861	808	146	-95.3	7.9E+01	2.0E+05	2.5E+00			4.8E-07	3.5E-07	1.1E-06				15%	-8.0	-7.7	-9.5
5,5,5',5'-tetramethyl-2,2'-bi-1,3,2-dioxaborinane	617-343-2	82530-64-1	82530641	3825	Reach_4451	809	199	16.1	2.9E+00	4.1E+02	7.1E+02			1.1E-06	3.5E-07	1.1E-06				16%	-7.0	-7.7	-9.6
calcium sulphidoacetate	249-881-5	29820-13-1	29820131	5825	Reach_2632	810	130	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.4	-7.7	-9.4
8-bromo-7-(but-2-yn-1-yl)-3-methyl-3,7-dihydro-1H-purine-2,6	203-870-1	111-44-4	111444	301	Reach_857	811	143	-34.4	1.4E+02	4.2E+03	3.6E+01			1.7E-08	3.5E-08	1.1E-07				16%	-6.8	-7.7	-9.6
2-methylbut-3-yn-2-ol	204-070-5	115-19-5	115195	339	Reach_939	812	84	-35.0	2.2E+03	2.5E+05	2.8E+00	13.6		1.1E-08	1.1E-06	3.5E-06				23%	-8.0	-7.7	-8.9
trans-4-aminocyclohexan-1-ol	616-451-7	77326-36-4	77326364	3731	Reach_4439	813	136	55.8	1.4E+00	5.0E+03	2.3E+01		13.7	1.1E-06	3.5E-07	1.1E-06				17%	-7.9	-7.7	-9.4
salicylamide	200-609-3	65-45-2	65452	784	Reach_76	814	137	118.0	4.0E+00	7.5E+03	1.1E+01	8.3		2.6E-07	3.5E-07	1.1E-06				17%	-8.0	-7.7	-9.4
potassium tert-butanolate	212-740-3	865-47-4	865474	6065	Reach_1569	815	112	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.4	-7.7	-9.4
(6R-trans)-7-amino-3-[[(5-methyl-1,3,4-thiadiazol-2-yl)thio]met	201-755-0	87-59-2	87592	978	Reach_311	816	121	29.1	1.6E+01	1.0E+03	1.5E+02		9	2.2E-09	3.5E-08	1.1E-07				16%	-6.6	-7.7	-9.6
N-(2,6-dimethylphenyl)pyridine-2-carboxamide	208-601-1	534-52-1	534521	682	Reach_1332	817	198	121.2	2.3E-04	4.7E+03	1.9E+02	4.2		2.2E-09	3.5E-08	1.1E-07				16%	-7.0	-7.7	-9.6
(6R-trans)-7-amino-3-chloro-8-oxo-5-thia-1-azabicyclo[4.2.0]oc	600-558-0	104358-16-9	104358169	1390	Reach_4068	818	236	58.9	4.6E-02	2.1E-01	1.5E+06			1.1E-06	1.1E-07	3.5E-07				16%	-6.6	-7.8	-9.6
4,6-dichloropyrimidine	224-698-3	4454-05-1	4454051	1269	Reach_2038	819	114	-45.3	2.8E+03	1.9E+04	7.6E+00			1.1E-06	1.1E-07	3.5E-07				16%	-8.0	-7.8	-9.1
nicotinic acid	200-441-0	59-67-6	59676	739	Reach_52	820	123	63.3	1.2E-02	4.1E+04	4.9E+00	1.96	9	6.3E-07	1.1E-07	3.5E-07				15%	-6.8	-7.8	-9.7
diallyl 2,2'-oxydiethyl dicarbonate	205-528-7	142-22-3	142223	1951	Reach_1175	821	274	43.4	8.6E-03	5.5E+02	3.5E+01			1.1E-06	1.1E-07	3.5E-07				14%	-7.6	-7.8	-9.8
Ethyl N-[3-amino-4-(methylamino)benzoyl]-N-pyridin-2-yl-β-ala	203-768-7	110-44-1	110441	1521	Reach_815	822	112	24.6	1.3E+00	2.2E+03	4.2E+01			3.5E-06	3.5E-07	1.1E-06				14%	-6.7	-7.8	-9.8
2-butoxyethyl acetate	203-933-3	112-07-2	112072	1573	Reach_887	823	160	-15.2	7.2E+01	3.2E+03	3.7E+01			1.1E-06	3.5E-07	1.1E-06				15%	-8.0	-7.8	-9.2
4-methylpentan-2-one	203-550-1	108-10-1	108101	229	Reach_728	824	100	-66.7	2.9E+03	1.0E+04	1.4E+01			9.4E-07	3.5E-07	1.1E-06				15%	-8.0	-7.8	-9.4
2-Chlorodibenzo[b,f][1,4]thiazepin-11(10H)-one	248-492-8	27489-62-9	27489629	576	Reach_2607	825	115	20.3	5.3E+00	5.7E+04	1.2E+00	15.7	4	2.0E-07	1.1E-06	3.5E-06				16%	-7.3	-7.8	-9.6
4-chlorobenzaldehyde	203-247-4	104-88-1	104881	171	Reach_631	826	141	8.7	1.4E+01	9.5E+02	2.2E+02			5.8E-07	1.1E-07	3.5E-07				15%	-8.0	-7.8	-9.1
propionaldehyde	204-623-0	123-38-6	123386	391	Reach_1047	827	58	-93.2	4.2E+04	2.0E+05	2.1E+00			4.5E-06	1.1E-06	3.5E-06				14%	-8.0	-7.8	-9.4
3-chloropropyltrimethoxysilane	219-787-9	2530-87-2	2530872	2430	Reach_1832	828	199	-3.7	4.5E+01	2.2E+03	3.6E+00			1.1E-07	3.5E-08	1.1E-07				19%	-8.0	-7.8	-9.1
4-phenylmorpholin-3-one	225-172-6	4698-11-7	4698117	1270	Reach_2056	829	223	126.2	1.4E-03	2.1E+01	2.2E+03		13.2	1.1E-06	1.1E-07	3.5E-07				14%	-7.6	-7.8	-9.8
bis(α,α-dimethylbenzyl) peroxide	201-279-3	80-43-3	80433	3791	Reach_262	830	270	103.6	1.0E-03	7.0E-01	7.6E+05			1.1E-06	1.1E-07	3.5E-07				19%	-7.8	-7.8	-9.4
tris(methylphenyl) phosphite	203-446-6	106-95-6	106956	204	Reach_685	831	121	-80.5	1.9E+04	3.5E+03	1.0E+02			1.6E-06	3.5E-07	1.1E-06				23%	-7.3	-7.8	-8.5
2-(trifluoromethyl)benzenesulfonamide	700-280-0	1869-24-5	1869245	2205	Reach_4839	832	225	87.7	7.7E-02	9.6E+02	2.1E+01	9.41		3.5E-07	3.5E-08	1.1E-07				16%	-8.0	-7.8	-9.6
disodium 4,4'-dinitrostilbene-2,2'-disulphonate	223-051-2	3709-43-1	3709431	5862	Reach_1985	833	474	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.4	-7.8	-9.4
(3-methacrylamidopropyl)trimethylammonium chloride	257-182-1	51410-72-1	51410721	5905	Reach_2773	834	221	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.5	-7.8	-9.4
hexan-1-ol	203-852-3	111-27-3	111273	294	Reach_850	835	102	-37.9	1.2E+02	1.1E+04	6.6E+01	15.9		3.9E-06	1.1E-06	3.5E-06				14%	-8.0	-7.8	-9.5
decan-1-ol	203-956-9	112-30-1	112301	325	Reach_896	836	158	7.9	1.5E+00	3.7E+01	6.2E+03	15.9		3.7E-06	1.1E-07	3.5E-07				15%	-8.0	-7.8	-9.4
607-864-3	607-864-3	26116-57-4	26116574	5802	Reach_4250	837	785	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.4	-7.8	-9.4
2,3-epoxypropyl phenyl ether	204-557-2	122-60-1	122601	381	Reach_1032	838	150	13.0	4.7E+00	1.1E+03	4.1E+01			1.6E-07	1.1E-07	3.5E-07				18%	-8.0	-7.8	-9.1
Bis (acetato-κO)[7-chloro-1-cyclopropyl-6-fluoro-4-(oxo-i	700-382-5	119618-67-6	119618676	1697	Reach_4883	839	410	173.4	2.3E-06		5.4E+01		15.6	3.5E-07	1.1E-07	3.5E-07				16%	-7.0	-7.8	-9.6
[(±)-(4-amino-2-hydroxy-4-oxobutyl)trimethylammonium] chlo	226-073-0	5261-99-4	5261994	5914	Reach_2088	840	197	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.5	-7.8	-9.4
3-aminopropan-1-ol	205-864-4	156-87-6	156876	494	Reach_1216	841	75	-15.4	2.1E+01	1.0E+06	7.6E-02	15.3	4	4.7E-07	1.1E-06	3.5E-06				15%	-7.6	-7.8	-9.6
bis(2-methoxyethyl) ether	203-924-4	111-96-6	111966	318	Reach_883	842	134	-39.0	4.0E+02	3.2E+05	3.3E-01			2.2E-09	1.1E-07	3.5E-07				23%	-8.0	-7.8	-8.8
2-chloro-N-methoxy-N-methylacetamide	201-141-2	78-77-3	78773	3757	Reach_207	843	137	-78.1	8.3E+03	1.2E+03	3.8E+02			3.5E-06	1.1E-06	3.5E-06				16%	-8.0	-7.8	-9.6
dimantine	204-694-8	124-28-7	124287	1790	Reach_1075	844	298	81.3	2.2E-02	7.5E-04	2.5E+08		3.9	1.1E-06	1.1E-07	3.5E-07				23%	-7.7	-7.8	-9.7
potassium hydrogen tartrate	212-769-1	868-14-4	868144	6070	Reach_1573	845	188	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.5	-7.8	-9.4
tetrafluoroethylene	204-126-9	116-14-3	116143	1645	Reach_951	846	100	-161.8	1.9E+06	2.8E+01	1.6E+01			3.5E-08	1.1E-08	3.5E-08				23%	-8.1	-7.8	-10.6
3-(trichlorosilyl)propiononitrile	213-986-4	1071-22-3	1071223	1455	Reach_1640	847	189	6.8	6.0E+01	1.1E+04	3.3E+01			3.5E-07	1.1E-07	3.5E-07				16%	-8.0	-7.8	-9.2
dexpanthenol	201-327-3	81-13-0	81130	3802	Reach_272	848	205	161.4	2.0E-06	1.3E+05	1.2E-02	13.2	15.5	1.1E-06	3.5E-07	1.1E-06				14%	-6.5	-7.8	-9.8
cyanoacetic acid	206-743-9	372-09-8	372098	2794	Reach_1257	849	85	38.0	4.7E+00	1.2E+06	1.7E-01	2.4		3.5E-06	3.5E-07	1.1E-06				14%	-6.6	-7.8	-9.8
diisopropylamine	200-855-1	75-26-3	75263	3660	Reach_135	850	123	-91.0	2.9E+04	2.7E+03	1.2E+02			1.1E-06	3.5E-07	1.1E-06				15%	-8.0	-7.8	-9.5
605-460-1	219-755-4	2524-04-1	2524041	1248	Reach_1829	851	189	-74.2	5.3E+01	5.6E+02	2.3E+02			3.5E-07	1.1E-07	3.5E-07				14%	-7.8	-7.8	-9.9
(3H)-benzofuran-2-one	209-052-0	553-86-6	553866	3169	Reach_1361	852	134	31.0	2.2E+00	2.6E+03	3.0E+00			1.1E-06	1.1E-07	3.5E-07				14%	-8.0	-7.8	-9.7
5-chloro-2-phenoxyaniline	204-125-3	116-11-0	116110	1644	Reach_950	853	72	-111.7	7.1E+04	2.1E+04	9.3E+00			1.1E-06	3.5E-07	1.1E-06				16%	-7.1	-7.8	-9.7
N-1-naphthylaniline	201-983-0	90-30-2	90302	1002	Reach_362	854	219	114.8	3.9E-03	1.8E+01	3.0E+04		13	6.2E-09	1.1E-08	3.5E-08				23%	-7.6	-7.8	-8.8
isopulegol	249-277-1	28874-51-3	28874513	5820	Reach_2625	855	151	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				21%	-8.0	-7.8	-9.1
2-chloronicotinic acid	220-937-0	2942-59-8	2942598	2566	Reach_1890	856	158	85.4	1.6E-01	2.0E+03	9.8E+00	2.89	15.9	1.1E-06	1.1E-07	3.5E-07				14%	-6.8	-7.8	-9.8
glyoxal	203-474-9	107-22-2	107222	217	Reach_701	857	58	-66.7	3.8E+04	4.7E+05	2.2E-02			4.7E-06	1.1E-06	3.5E-06				14%	-8.0	-7.8	-9.4
2,2'-bipyridyl	206-674-4	366-18-7	366187	2770	Reach_1252	858	156	77.8	3.8E-01	3.9E+03	2.4E+01		9.6	1.1E-06	1.1E-07	3.5E-07				14%	-6.9	-7.8	-9.8
phenothiazine	202-196-5	92-84-2	92842	4051	Reach_394	859	199	121.8	1.1E-04	3.3E+01	6.6E+03		13.2	1.1E-06	3.5E-07	1.1E-06				14%	-7.3	-7.8	-9.7
N-(hydroxymethyl)acrylamide	213-103-2	924-42-5	924425	4033	Reach_1593	860	101	69.5	2.7E-02	2.3E+05	1.5E-02	13.3	15.3	3.5E-06	3.5E-07	1.1E-06				14%	-6.5	-7.8	-9.8
sodium O,O-diethyl dithiophosphate	222-079-2	3338-24-7	3338247	5847	Reach_1950	861	208	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.5	-7.8	-9.4
octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine	220-260-0	2691-41-0	2691410	575	Reach_1855	862	296	182.9	3.2E-06	1.0E+06	6.6E+00			1.0E-07	3.5E-08	1.1E-07				19%	-6.9	-7.8	-9.4
sodium N-chlorobenzenesulphonamide	210-959-9	626-67-5	626675	769	Reach_1458	863	99	-38.5	3.7E+03	4.5E+04	2.5E+01									18%	-7.5	-7.8	-9.5
disodium adipate	204-682-2	124-12-9	124129	1785	Reach_1069	864	125	-10.8	3.7E+01	9.3E+01	6.3E+02									18%	-7.5	-7.8	-9.5
octanoic acid	204-677-5	124-07-2	124072	401	Reach_1066	865	144	48.4	6.5E+00	1.3E+03	1.1E+03	4.9		3.8E-06	3.5E-07	1.1E-06				14%	-7.8	-7.8	-9.8
N-(4-amino-2-ethoxyphenyl)acetamide	203-503-5	107-56-2	107562	1465	Reach_711	866	214	-59.5	3.7E+00	7.1E+01	1.2E+03	-0.1		3.5E-07	1.1E-07	3.5E-07				16%	-6.9	-7.8	-9.7
zinc methacrylate	236-144-8	13189-00-9	13189009	5665	Reach_2327	867	236	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.5	-7.8	-9.5
N-(2-methoxy-5-methylphenyl)acetamide	230-157-2	6962-44-3	6962443	3546	Reach_2215	868	179	118.3	3.4E-03	2.0E+03	1.4E+01	13.3	13.7	3.5E-07	1.1E-07	3.5E-07				16%	-7.2	-7.8	-9.7
619-874-5	619-874-5	42355-78-2	42355782	1242	Reach_4551	869	1101	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.5	-7.8	-9.5
nitrilotriacetic acid	205-355-7	139-13-9	139139	27	Reach_1142	870	191	296.6	9.5E-07	2.8E+04	1.5E-04	1.2	4.86	6.8E-09	1.1E-07	3.5E-07				23%	-6.9	-7.8	-8.8
chloroacetyl chloride	201-171-6	79-04-9	79049	910	Reach_225	871	113	-46.5	3.9E+03	1.5E+04	6.0E-01			8.1E-07	3.5E-08	1.1E-07				15%	-8.2	-7.8	-9.7
1-phenoxypropan-2-ol	212-222-7	770-35-4	770354	3730	Reach_1544	872	152	21.0	6.9E-01	2.9E+03	3.3E+01	14.9		1.1E-06	1.1E-07	1.1E-06				14%	-8.1	-7.8	-9.7
sodium N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy	217-461-0	1860-26-0	1860260	2200	Reach_1728	873	354	88.8	1.3E-03	5.0E-05	1.3E+10									18%	-7.5	-7.8	-9.5
3-(3-Amino-2-cyanophenoxy)-2,2-dimethyl-N-propylpropanam	226-467-2	5407-04-5	5407045	1184	Reach_2105	874	158	0.0												16%	-7.1	-7.8	-9.7
2-methylimidazole	211-765-7	693-98-1	693981	806	Reach_1509	875	82	35.5	9.2E-02	5.0E+04	4.1E+00	14.2	6	5.0E-07	3.5E-08	1.1E-07				15%	-7.0	-7.8	-9.8
600-314-3	606-907-3	22038-86-4	22038864	2315	Reach_4224	876	151	34.4	7.6E+00	6.1E+03	3.7E+01			1.1E-06	1.1E-07	3.5E-07				16%	-6.9	-7.8	-9.7
N,N-dimethyldocosylamine	244-433-5	21542-96-1	21542961	2298	Reach_2506	877	354	117.4	2.1E-04	5.0E-06	2.2E+10		3.9	1.1E-06	1.1E-07	3.5E-07				24%	-7.9	-7.8	-8.9

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
1,3,5-triazine-2,4,6(1H,3H,5H)-trithione, trisodium salt	241-749-5	17766-26-6	17766266	5742	Reach_2442	878	243	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.5	-7.8	-9.5
6-phenyl-1,3,5-triazine-2,4-diyldiamine	202-095-6	91-76-9	91769	4021	Reach_380	879	187	159.4	1.7E-05	7.0E+03	2.8E+01		9.6	3.5E-06	1.1E-07	1.1E-06				14%	-7.0	-7.8	-9.8
603-373-3	601-577-7	118969-29-2	118969292	5619	Reach_4093	880	342	0.0	0.0E+00	0.0E+00	0.0E+00		0	0.0E+00	0.0E+00	0.0E+00				22%	-7.2	-7.8	-8.9
2-chlorobenzothiazole	222-315-4	3423-28-7	3423287	2697	Reach_1958	881	167	46.1	3.5E+00	1.3E+04	2.2E+01		4.4	1.1E-06	1.1E-07	3.5E-07				16%	-7.0	-7.8	-9.7
3,5-xylidine	230-636-6	7235-40-7	7235407	3602	Reach_2232	882	537	237.5	2.4E-09	1.5E-10	4.2E+17			3.5E-07	3.5E-08	1.1E-07				16%	-8.0	-7.8	-9.6
benzylamine	246-376-1	24634-61-5	24634615	5792	Reach_2551	883	150	0.0												16%	-8.1	-7.8	-9.1
p-toluenesulphonyl isocyanate	223-810-8	4083-64-1	4083641	629	Reach_2011	884	197	104.0	1.3E-02	6.6E+02	2.2E+02			6.2E-08	1.1E-07	3.5E-07				20%	-7.9	-7.8	-9.2
cyclohex-1,4-ylenedimethanol	203-268-9	105-08-8	105088	1407	Reach_636	885	144	38.2	1.9E-02	1.7E+05	3.1E+01	15.6		3.5E-06	1.1E-06	3.5E-06				14%	-7.1	-7.8	-9.7
guaiacol	201-964-7	90-05-1	90051	3990	Reach_358	886	124	25.2	1.5E+01	3.9E+04	2.2E+01	10		1.1E-06	3.5E-07	1.1E-06				14%	-8.1	-7.8	-9.7
10,11-dihydro-5H-dibenz[b,f]azepine	601-145-8	111974-73-3	111974733	1566	Reach_4079	887	321	168.5	2.5E-06	7.1E-01	1.9E+05			3.5E-07	3.5E-08	1.1E-07				16%	-7.3	-7.8	-9.7
4-hydroxybenzoic acid	202-804-9	99-96-7	99967	1093	Reach_543	888	138	93.8	9.4E-04	1.2E+04	2.5E+01	4.6		1.4E-06	3.5E-07	1.1E-06				14%	-7.1	-7.8	-9.8
604-047-3	250-002-2	30018-16-7	30018167	5830	Reach_2641	889	443	0.0												16%	-7.4	-7.8	-9.7
geraniol	203-377-1	106-24-1	106241	186	Reach_661	890	154	-10.8	2.1E+00	3.4E+02	3.0E+03	15.5		5.8E-07	3.5E-07	1.1E-06				16%	-8.1	-7.8	-9.4
glycerol trinitrate	200-240-8	55-63-0	55630	702	Reach_24	891	227	50.2	3.6E+00	2.6E+04	3.2E+01			1.5E-06	3.5E-08	1.1E-07				14%	-8.1	-7.8	-9.9
2-octyldodecan-1-ol	226-242-9	5333-42-6	5333426	3096	Reach_2098	892	299	95.4	3.6E-05	7.5E-04	4.3E+08	15.9		1.1E-06	1.1E-07	3.5E-07				23%	-7.6	-7.8	-8.7
dodec-1-ene	203-968-4	112-41-4	112414	1588	Reach_905	893	168	-22.2	3.6E+01	5.3E-02	1.3E+06			3.5E-07	3.5E-08	1.1E-07				23%	-8.1	-7.8	-10.6
disodium 4,4'-bis[(4,6-dianilino-1,3,5-triazin-2-yl)amino]stilben	205-117-2	133-66-4	133664	5669	Reach_1124	894	937	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.5	-7.8	-9.5
2,9-dimethylanthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,	226-866-1	5521-31-3	5521313	3163	Reach_2121	895	418	349.8	3.6E-18	6.3E-03	1.5E+04		12.8	1.1E-07	3.5E-09	1.1E-08				19%	-7.2	-7.8	-9.4
hexahydro-2H-azepin-2-one, sodium salt	218-336-3	2123-24-2	2123242	5772	Reach_1759	896	135	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.5	-7.8	-9.5
trimethoxysilane	219-637-2	2487-90-3	2487903	563	Reach_1816	897	121	-81.4	1.1E+04	1.3E+05	6.0E-02			4.5E-07	3.5E-07	1.1E-06				16%	-8.1	-7.8	-9.3
mercaptoacetic acid	200-677-4	68-11-1	68111	798	Reach_90	898	92	18.8	5.5E+01	2.8E+05	1.1E+00	3.7		4.5E-06	3.5E-07	1.1E-06				14%	-6.7	-7.8	-9.8
tetramethylammonium chloride	200-880-8	75-57-0	75570	1235	Reach_152	899	110	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.5	-7.8	-9.5
trichloroethylene	201-167-4	79-01-6	79016	909	Reach_223	900	131	-77.2	9.7E+03	7.0E+02	3.0E+02			2.6E-08	3.5E-08	1.1E-07				23%	-8.2	-7.8	-10.4
isopropylamine	200-860-9	75-31-0	75310	855	Reach_138	901	59	-83.7	7.9E+04	2.1E+05	1.9E+00		4	4.1E-07	3.5E-07	1.1E-06				16%	-8.1	-7.8	-9.4
2-naphthol	205-182-7	135-19-3	135193	435	Reach_1129	902	144	67.7	2.2E-02	2.5E+02	4.9E+02	9.6		6.7E-07	3.5E-08	3.5E-07				15%	-8.0	-7.8	-9.7
glycerol	200-289-5	56-81-5	56815	716	Reach_30	903	92	19.4	1.1E-02	1.0E+06	2.2E-02	14.2		1.2E-06	1.1E-06	3.5E-06				14%	-6.9	-7.8	-9.8
2,4-dihydro-5-methyl-2-phenyl-3H-pyrazol-3-imine	203-776-0	110-53-2	110532	1522	Reach_816	904	151	-53.8	1.7E+03	1.7E+02	1.4E+03			3.5E-07	3.5E-08	1.1E-07				16%	-7.8	-7.8	-9.7
disodium 4,4'-diamino-9,9',10,10'-tetrahydro-9,9',10,10'-tetrac	227-877-4	6022-22-6	6022226	5946	Reach_2150	905	649	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.5	-7.8	-9.5
4-methoxybenzyl (6R,7R)-7-{[(2Z)-2-(5-amino-1,2,4-thiadiazol-3	700-025-3	102625-64-9	102625649	1348	Reach_4729	906	367	228.6	3.2E-09	4.4E+00	9.5E+02	11.9	8.88	1.1E-06	1.1E-07	3.5E-07				16%	-7.4	-7.8	-9.7
1-vinylimidazole	205-126-1	134-03-2	134032	5670	Reach_1126	907	198	0.0												16%	-8.0	-7.9	-9.7
2-(2H-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)phenol	221-573-5	3147-75-9	3147759	2626	Reach_1920	908	323	191.4	1.5E-07	3.1E-01	1.6E+06	10.3	15	3.5E-07	3.5E-08	1.1E-07				16%	-7.5	-7.9	-9.7
benzenesulphonyl chloride	202-636-6	98-09-9	98099	1066	Reach_497	909	177	61.2	3.3E+00	8.9E+02	8.7E+02			8.6E-07	3.5E-08	1.1E-07				15%	-8.1	-7.9	-9.5
methanesulphonic acid	200-898-6	75-75-2	75752	3683	Reach_159	910	96	25.8	3.6E+00	4.8E+05	4.2E-03	1.7		3.5E-06	1.1E-06	3.5E-06				14%	-6.8	-7.9	-9.8
itaconic acid	202-599-6	97-65-4	97654	4168	Reach_484	911	130	86.6	1.2E-02	4.5E+04	4.6E-01	3.87		3.5E-06	3.5E-07	1.1E-06				14%	-6.8	-7.9	-9.9
1-chloro-1,1-difluoroethane	200-891-8	75-68-3	75683	3681	Reach_158	912	101	-124.5	3.4E+05	2.0E+03	1.1E+02			3.5E-08	1.1E-08	1.1E-08				23%	-8.4	-7.9	-10.6
toluene-4-sulphonamide	200-741-1	70-55-3	70553	85	Reach_98	913	171	91.2	1.3E-02	2.0E+03	8.3E+00	10.1		4.3E-08	3.5E-08	1.1E-07				21%	-7.6	-7.9	-9.2
furan-2,5-dicarboxylic acid	221-800-8	3238-40-2	3238402	2650	Reach_1937	914	156	118.2	1.3E-05	8.8E+04	7.6E+00	2.63		3.5E-06	3.5E-07	1.1E-06				14%	-6.8	-7.9	-9.8
sodium 1,4-dicyclohexyl sulphonatosuccinate	245-629-3	23386-52-9	23386529	5785	Reach_2530	915	384	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.5	-7.9	-9.5
tetradecane	211-096-0	629-59-4	629594	3390	Reach_1468	916	198	1.4	4.9E+00	4.8E-03	1.7E+07			1.1E-06	1.1E-07	3.5E-07				23%	-8.0	-7.9	-10.5
(1S)-3-(dimethylamino)-1-(2-thienyl)propan-1-ol	608-570-8	31024-26-7	31024267	2616	Reach_4278	917	147	-12.1	3.8E+02	2.2E+04	2.2E+01		3.69	3.5E-06	1.1E-06	3.5E-06				14%	-6.9	-7.9	-10.0
diisobutyl phthalate	201-553-2	84-69-5	84695	962	Reach_289	918	278	17.6	3.2E-01	3.1E+01	2.9E+04			8.8E-07	1.1E-07	3.5E-07				17%	-8.1	-7.9	-9.4
10-methoxy-5H-dibenz[b,f]azepine	202-447-9	95-75-0	95750	1038	Reach_440	919	161	3.6	3.1E+01	3.6E+01	6.8E+03			2.7E-09	1.1E-08	3.5E-08				14%	-7.4	-7.9	-9.9
613-175-9	700-035-8	6246-48-6	6246486	3371	Reach_4733	920	153	-5.5	1.8E+01	8.2E+03	2.9E+03		4.2	1.1E-06	1.1E-07	1.1E-06				16%	-7.6	-7.9	-9.7
heptanoic acid	203-838-7	111-14-8	111148	293	Reach_845	921	130	37.5	1.6E+01	4.0E+03	3.5E+02	4.9		3.9E-06	3.5E-07	1.1E-06				14%	-7.8	-7.9	-9.8
decamethylenediamine	211-471-9	646-25-3	646253	3440	Reach_1484	922	172	59.6	7.1E-01	1.1E+03	2.0E+02		3.2	3.5E-07	3.5E-08	1.1E-07				16%	-8.1	-7.9	-9.6
611-084-9	211-519-9	657-27-2	657272	5975	Reach_1489	923	183	0.0												16%	-7.1	-7.9	-9.7
sodium 1-amino-4-bromo-9,10-dioxoanthracene-2-sulphonate	228-391-5	6258-06-6	6258066	5584	Reach_2158	924	404	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.6	-7.9	-9.5
4,4'-isopropylidenedicyclohexanol	201-244-2	80-04-6	80046	931	Reach_253	925	240	102.7	6.8E-05	9.0E+01	3.5E+04	15.7		2.6E-08	3.5E-08	1.1E-07				22%	-7.5	-7.9	-9.0
pyrene	204-927-3	129-00-0	129000	21	Reach_1114	926	202	119.9	4.6E-05	2.8E-02	8.5E+04			2.2E-09	3.5E-09	1.1E-08				24%	-8.1	-7.9	-8.8
N-phenylpiperazine	700-095-5	203448-76-4	203448764	2262	Reach_4759	927	276	63.3	1.4E-01	1.4E+02	4.8E+01			3.5E-06	3.5E-07	1.1E-06				16%	-7.2	-7.9	-9.7
bis(2-ethylhexyl) sebacate	204-558-8	122-62-3	122623	1755	Reach_1033	928	427	51.0	2.6E-04	4.9E-04	1.2E+10			1.1E-06	1.1E-07	3.5E-07				23%	-7.9	-7.9	-8.7
acetoacetanilide	202-996-4	102-01-2	102012	1334	Reach_587	929	177	123.7	4.1E-03	7.7E+03	1.0E+01	10.7	13.4	1.1E-06	1.1E-07	3.5E-07				14%	-6.9	-7.9	-9.9
bis(2-ethylhexyl) hydrogen phosphate	206-056-4	298-07-7	298077	592	Reach_1227	930	322	86.3	2.4E-05	6.0E-01	1.2E+06	1.5		2.6E-08	3.5E-08	1.1E-07				22%	-7.8	-7.9	-9.1
sodium butanolate	219-144-2	2372-45-4	2372454	5787	Reach_1787	931	96	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.6	-7.9	-9.5
potassium trifluoroacetate	220-877-5	2923-16-2	2923162	5822	Reach_1887	932	152	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.6	-7.9	-9.5
(Z)-octadec-9-enol	205-597-3	143-28-2	143282	1962	Reach_1192	933	268	85.4	2.0E-03	2.7E-03	3.2E+07	15.9		1.1E-06	3.5E-07	1.1E-06				22%	-7.9	-7.9	-9.7
potassium carbamoylcarbamate	247-728-7	26479-35-6	26479356	5805	Reach_2583	934	142	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.6	-7.9	-9.5
N-(2-bromo-4-fluorophenyl)acetamide	700-330-1	433733-92-7	433733927	2909	Reach_4864	935	240	176.7	5.4E-08	9.7E+04	2.8E-01	14.4		3.5E-06	3.5E-07	1.1E-06				16%	-7.8	-7.9	-9.7
zinc dilactate	240-178-9	16039-53-5	16039535	5730	Reach_2409	936	244	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.6	-7.9	-9.5
α,α,α,4-tetrachlorotoluene	210-258-8	611-19-8	611198	3326	Reach_1419	937	161	3.4	2.0E+01	5.1E+01	2.8E+03			1.1E-07	1.1E-08	3.5E-08				22%	-8.2	-7.9	-9.9
mequinol	205-769-8	150-76-5	150765	483	Reach_1204	938	124	25.2	1.1E+00	6.7E+04	3.9E+01	10.1		7.2E-07	3.5E-07	1.1E-06				15%	-7.8	-7.9	-9.8
5-amino-2,4,6-triiodoisophthalic acid	252-575-4	35453-19-1	35453191	2736	Reach_2691	939	559	231.7	2.0E-09	1.7E+00	1.4E+02	1.31		3.5E-06	3.5E-07	1.1E-06				14%	-7.1	-7.9	-9.8
N-(cyclohexylthio)phthalimide	241-774-1	17796-82-6	17796826	2153	Reach_2444	940	261	197.8	3.5E-07	1.0E+02	5.8E+03			1.1E-06	1.1E-07	3.5E-07				15%	-7.1	-7.9	-9.7
4-chloro-3-nitrobenzoic acid	603-565-7	132335-44-5	132335445	1857	Reach_4125	941	185	69.7	1.7E-02	2.4E+04	1.0E+01	15.4		1.1E-06	3.5E-08	1.1E-07				14%	-7.1	-7.9	-10.0
1,3-diphenyl-2-thiourea	203-004-2	102-08-9	102089	151	Reach_589	942	228	124.6	3.7E-04	3.0E+01	1.6E+03	11.4	13	5.2E-09	1.1E-07	3.5E-07				23%	-7.8	-7.9	-8.9
2,3,5-trimethylhydroquinone	206-441-7	342-25-6	342256	2695	Reach_1239	943	218	74.7	1.3E-01	1.7E+01	3.5E+03			1.1E-06	3.5E-08	1.1E-07				16%	-7.7	-7.9	-9.7
(2E,4R)-5-(biphenyl-4-yl)-4-[(tert-butoxycarbonyl)amino]-2-me	605-866-9	179688-26-7	179688267	2160	Reach_4183	944	343	170.6	1.1E-05	9.3E+01	1.7E+01			1.1E-06	1.1E-07	3.5E-07				16%	-7.4	-7.9	-9.7
4,4'-[(isopropylidene)bis(p-phenyleneoxy)]diphthalic dianhydri	253-781-7	38103-06-9	38103069	2816	Reach_2716	945	520	285.4	4.4E-13	3.7E-04	7.4E+08			1.1E-06	1.1E-07	3.5E-07				23%	-7.6	-7.9	-8.5
tris(2-ethylhexyl) phosphate	201-116-6	78-42-2	78422	895	Reach_199	946	435	87.0	8.1E-05	1.9E-04	3.1E+09			1.6E-08	1.1E-07	3.5E-07				24%	-7.8	-7.9	-8.9
17-hydroxypregna-4,9(11)-diene-3,20-dione	247-768-5	26537-19-9	26537199	2475	Reach_2586	947	192	34.6	2.6E+00	4.1E+01	5.5E+03			1.1E-06	1.1E-07	3.5E-07				16%	-7.1	-7.9	-9.7
bromoacetic acid	201-175-8	79-08-3	79083	912	Reach_228	948	139	29.2	1.7E+01	8.5E+04	2.7E+00	2.9		3.6E-07	3.5E-07	1.1E-06				16%	-7.1	-7.9	-9.7
1-(3-chlorophenyl)-4-(3-chloropropyl)piperazinium chloride	258-038-0	52605-52-4	52605524	5913	Reach_2785	949	310	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.6	-7.9	-9.6
iohexol	266-164-2	66108-95-0	66108950	80	Reach_2877	950	821	349.8	5.4E-27	6.4E-01	1.5E-03	11.8		1.1E-07	1.1E-07	3.5E-07				19%	-7.0	-7.9	-9.5
4-[[4-(aminocarbonyl)phenyl]azo]-N-(2-ethoxyphenyl)-3-hydro	220-509-3	2786-76-7	2786767	2520	Reach_1868	951	454	327.1	1.9E-17	1.5E-01	1.1E+06	9.46	14.9	3.5E-07	1.1E-08	3.5E-08				16%	-7.6	-7.9	-9.8
604-471-9	604-471-9	14543-49-8	14543498	1986	Reach_4155	952	140	-40.4	2.7E+02	5.8E+01	1.4E+03			1.1E-06	1.1E-07	3.5E-07				19%	-8.2	-7.9	-10.5

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
citronellol	203-375-0	106-22-9	106229	185	Reach_659	953	156	-12.2	2.3E+00	3.5E+02	3.6E+03	15.9		4.1E-07	3.5E-07	1.1E-06				16%	-8.2	-7.9	-9.4
2-(isopropylthio)-3-(2,2,2-trifluoroethoxy)pyridine	206-887-2	393-52-2	393522	2838	Reach_1264	954	159	7.6	3.6E+01	5.2E+03	4.4E+01			1.1E-06	3.5E-07	1.1E-06				16%	-7.4	-7.9	-9.8
3-hydroxy-N-(o-tolyl)-4-[(2,4,5-trichlorophenyl)azo]naphthalen	229-440-3	6535-46-2	6535462	3451	Reach_2193	955	485	290.2	1.1E-14	1.7E-04	1.6E+09	9.24		3.5E-08	1.1E-08	3.5E-08				24%	-7.9	-7.9	-8.5
p-phenetidine	205-855-5	156-43-4	156434	2048	Reach_1213	956	137	39.6	2.9E+00	4.7E+03	4.5E+01		8.6	1.1E-06	1.1E-07	3.5E-07				14%	-7.6	-7.9	-9.9
cyclododeca-1,5,9-triene	225-533-8	4904-61-4	4904614	648	Reach_2067	957	162	-15.2	9.8E+00	7.5E-01	3.0E+05			1.6E-08	1.1E-07	3.5E-07				24%	-8.2	-7.9	-10.4
2-[(p-aminophenyl)sulphonyl]ethyl hydrogensulphate	219-669-7	2494-89-5	2494895	2409	Reach_1820	958	281	203.6	1.2E-09	5.2E+03	2.1E-04	-3.44	12.6	1.1E-06	1.1E-07	1.1E-06				14%	-6.7	-7.9	-9.9
potassium 1,2-bis(2-ethylhexyloxycarbonyl)ethanesulphonate	231-308-5	7491-09-0	7491090	6023	Reach_2256	959	461	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.6	-7.9	-9.6
naphthalene-1,8-dicarboxylic anhydride	201-380-2	81-84-5	81845	3816	Reach_280	960	198	92.9	5.5E-05	1.1E+02	1.7E+03			1.1E-06	3.5E-08	1.1E-07				15%	-7.2	-7.9	-9.8
620-313-1	221-738-1	3217-00-3	3217003	2643	Reach_1933	961	166	100.4	9.1E-03	1.0E+06	2.2E-02			3.5E-06	3.5E-07	1.1E-06				17%	-7.3	-7.9	-9.7
sodium dimethyl 5-sulphonatoisophthalate	223-578-8	3965-55-7	3965557	5872	Reach_2004	962	296	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.6	-7.9	-9.6
bis(dibutyldithiocarbamato-S,S')copper	237-695-7	13927-71-4	13927714	5685	Reach_2351	963	472	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.6	-7.9	-9.6
ethyl 2-cyano-2-phenyl-butanoate	611-342-0	55974-25-9	55974259	3183	Reach_4356	964	220	89.2	2.2E-02	2.2E+02	1.9E+03			1.1E-06	1.1E-07	3.5E-07				16%	-8.2	-7.9	-9.7
2,2-bis(allyloxymethyl)butan-1-ol	211-661-1	682-09-7	682097	3510	Reach_1499	965	214	55.2	2.1E-02	3.0E+02	7.4E+01	15.1		1.1E-06	1.1E-07	3.5E-07				14%	-8.1	-7.9	-9.9
603-923-2	603-923-2	135590-91-9	135590919	436	Reach_4133	966	373	149.9	4.4E-04	2.4E+00	6.6E+04			8.8E-08	1.1E-07	3.5E-07				21%	-8.0	-7.9	-9.3
600-024-7	231-501-4	7597-60-6	7597606	3691	Reach_2265	967	198	195.2	5.1E-07	7.5E+04	4.4E-02									18%	-7.6	-7.9	-9.6
2,2,4,4-tetramethyl-7-oxa-3,20-diazadispiro[5.1.11.2]henicosar	219-542-6	2458-08-4	2458084	1246	Reach_1813	968	407	231.7	2.3E-12	3.0E+01	5.1E+03									18%	-7.6	-7.9	-9.6
N-methylformamide	204-624-6	123-39-7	123397	392	Reach_1048	969	59	28.2	4.9E+01	1.0E+06	7.2E-02	15.1	14	5.5E-07	1.1E-07	3.5E-07				15%	-7.8	-7.9	-9.9
610-954-5	200-261-2	56-18-8	56188	3188	Reach_25	970	131	40.5	1.1E+01	1.0E+06	7.1E-02									18%	-7.6	-7.9	-9.6
amantadine hydrochloride	700-238-1	132900-75-5	132900755	1861	Reach_4815	971	617	288.4	2.7E-13	1.0E-04	1.7E+08									18%	-7.6	-7.9	-9.6
calcium di(acetate)	259-393-4	54914-37-3	54914373	3156	Reach_2803	972	278	40.8	8.7E-02	1.7E+00	1.4E+07									18%	-7.6	-7.9	-9.6
3-(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)propanal	204-092-5	115-46-8	115468	1637	Reach_942	973	267	151.2	1.1E-06	4.6E+02	2.8E+03		3.5	1.1E-06	1.1E-07	3.5E-07				14%	-6.9	-7.9	-10.0
p-menthane-1,8-diol	201-288-2	80-53-5	80535	3793	Reach_265	974	172	49.4	2.8E-02	1.4E+05	2.1E+02	15.6		1.1E-06	1.1E-07	3.5E-07				15%	-7.2	-7.9	-9.9
decyl oleate	222-981-6	3687-46-5	3687465	2782	Reach_1982	975	423	161.3	1.7E-06	2.3E-07	2.8E+12			1.1E-06	1.1E-07	3.5E-07				24%	-8.2	-7.9	-8.4
2-(methylamino)ethanol, compound with sulphur dioxide	244-311-1	21282-97-3	21282973	2288	Reach_2504	976	214	-23.3	2.8E+00	7.1E+03	1.7E+00									18%	-7.6	-7.9	-9.6
α,α,α-trichlorotoluene	210-275-0	611-70-1	611701	3328	Reach_1421	977	148	2.0	1.7E+01	3.5E+02	3.8E+02			3.5E-07	1.1E-07	3.5E-07				23%	-8.2	-7.9	-9.8
2,4,4-trimethylpentene	246-690-9	25167-70-8	25167708	2420	Reach_2561	978	112	-84.5	5.5E+03	4.3E+00	1.2E+04			1.1E-07	3.5E-08	1.1E-07				23%	-8.2	-7.9	-10.7
chlorodimethylsilane	213-912-0	1066-35-9	1066359	1440	Reach_1637	979	94	-124.7	7.3E+04	9.6E+03	8.5E+01			3.5E-09	3.5E-09	3.5E-09				24%	-8.4	-7.9	-10.5
2-morpholinoethanol	605-539-0	169115-74-6	169115746	5737	Reach_4178	980	194	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				21%	-7.4	-7.9	-9.2
tetradec-1-ene	214-306-9	1120-36-1	1120361	1569	Reach_1657	981	196	0.1	1.4E+01	6.7E-03	1.2E+07			3.5E-07	3.5E-08	1.1E-07				23%	-8.1	-7.9	-10.5
butane-1,3-diol	203-529-7	107-88-0	107880	1470	Reach_718	982	90	-21.1	4.3E+00	1.0E+06	5.1E-01	15.3		3.5E-06	1.1E-06	3.5E-06				14%	-7.3	-7.9	-9.9
2,9-bis(3,5-dimethylphenyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoc	225-590-9	4948-15-6	4948156	2983	Reach_2068	983	599	349.8	1.6E-23	7.8E-08	2.3E+07		12.8	1.1E-07	3.5E-09	1.1E-08				19%	-7.8	-7.9	-9.5
2,5-dimethylhexane-2,5-diol	203-731-5	110-03-2	110032	1513	Reach_802	984	146	19.3	5.8E-01	1.5E+05	3.3E+01	15.6		1.1E-06	3.5E-07	1.1E-06				14%	-7.5	-7.9	-9.8
1,2,4-trichlorobenzene	204-429-6	120-83-2	120832	363	Reach_1004	985	163	46.8	8.8E+00	3.6E+03	6.3E+02			2.2E-09	3.5E-08	1.1E-07				24%	-8.2	-7.9	-9.9
6-amino-1,3-dimethyluracil	202-046-9	91-17-8	91178	1005	Reach_371	986	138	-28.9	1.3E+02	1.9E+00	1.6E+04			5.8E-09	1.1E-07	3.5E-07				14%	-6.9	-7.9	-10.1
strontium 3-hydroxy-4-[(4-methyl-2-sulphonatophenyl)azo]-2-r	277-552-6	73612-29-0	73612290	6016	Reach_2939	987	472	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.6	-7.9	-9.6
methyl stearate	203-990-4	112-61-8	112618	1595	Reach_916	988	299	81.6	4.4E-03	9.1E-03	1.7E+08			1.1E-06	1.1E-07	3.5E-07				23%	-7.8	-7.9	-9.5
7a-ethyldihydro-1H,3H,5H-oxazolo[3,4-c]oxazole	231-810-4	7747-35-5	7747355	880	Reach_2272	989	143	15.4	9.9E+01	2.8E+05	2.5E+00		8	1.9E-07	1.1E-07	3.5E-07				17%	-7.9	-7.9	-9.6
lactic acid	200-018-0	50-21-5	50215	654	Reach_4	990	90	22.7	3.8E+00	7.7E+05	2.2E-01	3.8		4.7E-07	3.5E-07	3.5E-07				15%	-6.9	-7.9	-9.9
1,2,3,6-tetrahydrophthalimide	201-602-8	85-40-5	85405	3888	Reach_293	991	151	172.1	1.6E-05	5.8E+04	2.0E+00	9.3		3.5E-06	1.1E-07	3.5E-07				14%	-6.8	-7.9	-10.2
3-((5-(3-(Dodecanoyloxy)-2,2-dimethylpropylideneamino)-1,3,3	700-071-4	932742-30-8	932742308	4067	Reach_4751	992	703	273.1	1.2E-12	1.7E-10	9.3E+16		7.55	1.1E-06	1.1E-07	3.5E-07				24%	-8.2	-8.0	-5.7
(+)-menthol	239-387-8	15356-60-2	15356602	486	Reach_2385	993	156	-5.9	1.0E+00	9.4E+02	2.4E+03	16		3.2E-07	1.1E-07	3.5E-07				17%	-8.2	-8.0	-9.6
2-acrylamido-2-methylpropanesulphonic acid	239-268-0	15214-89-8	15214898	2021	Reach_2378	994	207	160.8	9.0E-07	4.1E+04	6.5E-03	1.19	15.9	3.5E-06	1.1E-06	3.5E-06				14%	-6.7	-8.0	-9.9
dilauroyl peroxide	203-326-3	105-74-8	105748	1419	Reach_648	995	399	56.4	2.7E-04	1.3E-04	2.2E+10			1.1E-06	1.1E-07	3.5E-07				24%	-8.1	-8.0	-8.9
carbon tetrachloride	200-262-8	56-23-5	56235	710	Reach_26	996	154	-58.4	1.3E+04	3.9E+02	2.8E+02			3.9E-08	1.1E-08	3.5E-08				23%	-8.4	-8.0	-10.6
2-propylvaleric acid	202-777-3	99-66-1	99661	1091	Reach_536	997	144	37.7	1.1E+01	5.1E+03	9.1E+02	4.9		1.6E-06	1.1E-07	3.5E-07				14%	-7.8	-8.0	-10.0
2-chloro-5-(trifluoromethyl)pyridine	257-856-5	52334-81-3	52334813	3058	Reach_2781	998	182	3.3	3.6E+02	5.4E+02	2.6E+02		15.7	3.5E-07	3.5E-08	1.1E-07				16%	-7.3	-8.0	-9.9
3-acetamido-5-amino-4-hydroxybenzenesulphonic acid	254-879-2	40306-75-0	40306750	2857	Reach_2730	999	246	220.8	5.8E-11	9.6E+01	3.5E-04	-0.27	10.8	1.1E-06	3.5E-08	1.1E-07				14%	-6.8	-8.0	-10.2
2-nitro-4-(trifluoromethyl)benzonitrile	212-298-1	778-94-9	778949	3743	Reach_1545	1000	216	81.5	1.8E-01	1.6E+02	2.1E+02			1.1E-06	3.5E-08	1.1E-07				15%	-8.2	-8.0	-9.8
N,N-dibutylformamide	202-546-7	96-93-5	96935	4156	Reach_471	1001	234	191.0	1.1E-08	2.8E+03	6.8E-03		12.3	3.5E-06	1.1E-07	3.5E-07				17%	-8.2	-8.0	-9.6
2-sec-butylphenol	201-933-8	89-72-5	89725	993	Reach_350	1002	150	38.6	5.3E+00	9.6E+02	2.9E+03	10.8		3.3E-08	1.1E-07	3.5E-07				22%	-8.2	-8.0	-9.2
2'-methylacetoacetanilide	202-267-0	93-68-5	93685	4078	Reach_405	1003	191	134.7	1.4E-03	7.9E+02	9.8E+00	10.7	13.4	1.1E-06	3.5E-07	1.1E-06				14%	-7.1	-8.0	-9.9
617-448-3	230-437-4	7139-02-8	7139028	1288	Reach_2226	1004	367	201.7	1.9E-07	1.2E-01	2.8E+05			3.5E-07	3.5E-08	1.1E-07				16%	-7.3	-8.0	-9.7
2-chloro-3-methyl-4-(methylsulfonyl)benzoic acid	205-451-9	141-05-9	141059	454	Reach_1156	1005	172	-72.3	2.4E+01	3.6E+03	1.6E+02			1.2E-06	3.5E-07	1.1E-06				14%	-7.1	-8.0	-10.0
600-451-9	205-844-5	155-41-9	155419	5717	Reach_1212	1006	398	0.0												16%	-7.4	-8.0	-9.7
docosanoic acid	204-010-8	112-85-6	112856	1608	Reach_927	1007	341	158.7	6.5E-05	2.0E-04	8.1E+09	4.9		1.1E-06	1.1E-07	3.5E-07				21%	-8.0	-8.0	-9.2
dipotassium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4	268-144-9	68015-77-0	68015770	5992	Reach_2896	1008	421	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.7	-8.0	-9.6
propylene carbonate	203-572-1	108-32-7	108327	1483	Reach_741	1009	102	19.6	5.6E+00	9.6E+02	1.2E+00			3.5E-06	3.5E-07	1.1E-06				14%	-8.2	-8.0	-9.8
bronopol	211-089-2	629-40-3	629403	771	Reach_1466	1010	136	42.6	8.2E-01	1.1E+03	2.1E+01	0		1.1E-08	1.1E-07	3.5E-07				22%	-7.5	-8.0	-9.1
4-(vinyloxy)butan-1-ol	241-793-5	17832-28-9	17832289	2154	Reach_2445	1011	116	-21.7	3.3E+01	1.0E+05	2.7E+00	15.9		1.1E-06	3.5E-07	1.1E-06				14%	-8.2	-8.0	-9.9
diammonium dihydrogen ethylenediaminetetraacetate	244-063-4	20824-56-0	20824560	1204	Reach_2499	1012	326	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.7	-8.0	-9.6
dimethyl [3-[(hydroxymethyl)amino]-3-oxopropyl]phosphonate	243-528-9	20120-33-6	20120336	2250	Reach_2488	1013	211	84.2	1.7E-05	3.2E+05	8.1E-04	12.7		1.1E-06	1.1E-07	1.1E-06				14%	-6.9	-8.0	-10.1
barium 4-[(5-chloro-4-methyl-2-sulphonatophenyl)azo]-3-hydr	231-494-8	7585-41-3	7585413	6029	Reach_2264	1014	556	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.7	-8.0	-9.6
triphenyl phosphite	202-908-4	101-02-0	101020	140	Reach_572	1015	310	143.8	1.0E-02	9.8E-01	4.2E+06			8.4E-08	3.5E-08	1.1E-07				23%	-8.0	-8.0	-9.1
sodium D-glycero-D-gulo-heptonate	235-849-8	13007-85-7	13007857	5656	Reach_2317	1016	248	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.7	-8.0	-9.6
trichloro(phenyl)silane	202-640-8	98-13-5	98135	1067	Reach_500	1017	212	5.8	4.6E+01	1.4E+03	4.0E+03			2.9E-08	3.5E-08	1.1E-07				22%	-8.3	-8.0	-9.3
vanillin	204-465-2	121-33-5	121335	369	Reach_1011	1018	152	71.6	6.0E-02	6.6E+03	1.1E+01	7.3		6.4E-07	3.5E-07	1.1E-06				15%	-7.6	-8.0	-9.9
1,5-naphthylene diisocyanate	221-641-4	3173-72-6	3173726	2631	Reach_1926	1019	210	76.8	4.6E-03	4.2E+02	2.3E+04			1.1E-06	1.1E-07	3.5E-07				16%	-7.8	-8.0	-9.8
β,β-carotene	226-897-0	5537-71-3	5537713	3168	Reach_2123	1020	175	109.8	3.7E-03	9.2E+02	7.2E+01			3.5E-06	3.5E-07	1.1E-06				24%	-8.2	-8.0	-6.0
coumarin	202-086-7	91-64-5	91645	1008	Reach_377	1021	146	33.3	8.8E-02	1.4E+03	3.2E+01			6.2E-07	3.5E-07	1.1E-06				15%	-8.1	-8.0	-9.8
2-(morpholinothio)benzothiazole	244-017-3	20769-85-1	20769851	2273	Reach_2498	1022	230	16.8	3.8E+02	5.2E+02	6.8E+00			1.1E-06	3.5E-07	1.1E-06				14%	-7.6	-8.0	-10.0
dimethyl methylphosphonate	212-052-3	756-79-6	756796	3680	Reach_1526	1023	124	-48.3	1.2E+02	7.1E+04	2.6E-01			1.1E-06	1.1E-07	1.1E-06				14%	-8.2	-8.0	-9.8
1-bromo-3-chloropropane	204-371-1	120-12-7	120127	358	Reach_989	1024	178	78.1	2.9E-04	6.6E-01	2.2E+04			4.2E-09	1.1E-08	3.5E-08				23%	-8.3	-8.0	-9.9
2,2'-[oxybis(methylene)]bis[2-ethylpropane-1,3-diol]	245-509-0	23235-61-2	23235612	2348	Reach_2529	1025	250	147.3	4.7E-07	3.0E+06	2.0E-01	14.6		1.1E-06	3.5E-07	1.1E-06				14%	-6.9	-8.0	-10.1
dipropylamine	205-565-9	142-84-7	142847	464	Reach_1181	1026	101	-54.3	3.3E+03	7.2E+04	6.2E+01		3	4.9E-07	3.5E-07	3.5E-07				16%	-8.2	-8.0	-9.3
2-(4-tert-butylbenzyl)propionaldehyde	201-289-8	80-54-6	80546	3794	Reach_266	1027	204	46.3	4.8E-01	3.9E+00	2.3E+04			3.5E-07	3.5E-08	1.1E-07				18%	-8.3	-8.0	-9.4

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
N-(2-benzylphenyl)-2-chloroacetamide	239-784-6	15687-27-1	15687271	493	Reach_2393	1028	206	94.2	2.5E-02	2.8E+01	6.2E+03	4.3		1.7E-08	1.1E-07	3.5E-07				14%	-7.4	-8.0	-10.0
triisodecyl benzene-1,2,4-tricarboxylate	253-138-0	36631-30-8	36631308	2771	Reach_2701	1029	631	246.0	2.1E-11	1.3E-07	3.5E+14			1.1E-06	1.1E-07	3.5E-07				24%	-8.2	-8.0	-7.6
4-chloro-4'-hydroxybenzophenone	255-627-4	42019-78-3	42019783	2886	Reach_2748	1030	233	126.7	2.7E-04	2.6E+01	2.0E+03	8.08		1.1E-07	3.5E-08	1.1E-07				19%	-8.0	-8.0	-9.5
2-vinylpyridine	202-879-8	100-69-6	100696	1309	Reach_569	1031	105	-15.2	3.4E+02	3.3E+05	5.1E+01		9.1	1.1E-06	1.1E-07	3.5E-07				14%	-7.5	-8.0	-10.0
619-326-5	600-314-3	102445-69-2	102445692	1342	Reach_4059	1032	425	209.0	1.6E-10	2.4E+00	1.8E+02	13.5		3.5E-07	3.5E-08	1.1E-07				14%	-6.8	-8.0	-10.2
sodium p-[(4,6-dichloro-1,3,5-triazin-2-yl)amino]benzenesulph	223-989-2	4156-21-2	4156212	5880	Reach_2017	1033	343	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.7	-8.0	-9.7
diethylamine	203-716-3	109-89-7	109897	5	Reach_796	1034	73	-79.7	3.1E+04	4.2E+05	6.5E+00		3.1	5.0E-07	3.5E-07	1.1E-06				16%	-8.3	-8.0	-9.3
601-577-7	243-317-1	19794-93-5	19794935	2243	Reach_2485	1035	372	211.5	1.1E-06	1.1E+01	1.6E+03									18%	-7.7	-8.0	-9.7
2-[(4-methoxy-2-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxol	229-419-9	6528-34-3	6528343	3450	Reach_2192	1036	386	241.6	4.3E-10	8.0E+00	9.8E+02	8.57	14	3.5E-07	3.5E-08	1.1E-07				16%	-7.2	-8.0	-9.8
tetramethylenediamine	203-782-3	110-60-1	110601	1524	Reach_819	1037	88	0.9	3.1E+02	1.0E+06	2.3E-01		3.39	3.5E-06	3.5E-07	1.1E-06				14%	-8.2	-8.0	-10.0
dibenzyl ether	203-118-2	103-50-4	103504	1369	Reach_608	1038	198	55.7	2.9E-01	1.7E+01	3.0E+03			1.1E-06	1.1E-07	3.5E-07				15%	-8.3	-8.0	-9.5
sodium hydrogen N-(1-oxododecyl)-L-glutamate	249-958-3	29923-31-7	29923317	5828	Reach_2639	1039	351	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.7	-8.0	-9.7
3-chloroaniline	226-724-9	5459-04-1	5459041	1276	Reach_2114	1040	230	20.4	3.9E-01	2.0E+04	1.9E-02		0	3.5E-06	3.5E-07	1.1E-06				23%	-7.8	-8.0	-9.0
glutaral	203-856-5	111-30-8	111308	296	Reach_852	1041	100	-29.9	2.5E+02	6.1E+05	6.6E-01			4.4E-06	3.5E-07	1.1E-06				14%	-8.2	-8.0	-10.0
valeric acid	203-677-2	109-52-4	109524	256	Reach_774	1042	102	14.8	9.6E+01	3.5E+04	3.6E+01	4.9		4.1E-06	3.5E-07	1.1E-06				14%	-7.7	-8.0	-10.0
2,2-bis[[(2-ethyl-1-oxohexyl)oxy]methyl]propane-1,3-diyl bis(2-	230-743-8	7299-99-2	7299992	3611	Reach_2234	1043	641	220.2	2.7E-10	4.5E-07	2.2E+12			1.1E-06	1.1E-07	3.5E-07				24%	-8.2	-8.0	-8.5
2-decyltetradecanol	261-385-0	58670-89-6	58670896	3252	Reach_2831	1044	355	131.5	6.5E-07	5.4E-06	3.9E+10	15.9		1.1E-06	1.1E-07	3.5E-07				24%	-8.1	-8.0	-8.6
o-(trifluoromethyl)benzamide	206-637-2	360-64-5	360645	2756	Reach_1251	1045	189	90.2	8.0E-02	4.2E+02	9.3E+00	12.7		1.1E-06	1.1E-07	3.5E-07				14%	-8.2	-8.0	-10.0
pentan-3-one	202-490-3	96-22-0	96220	1048	Reach_455	1046	86	-67.7	5.3E+03	1.1E+05	5.6E+00			9.4E-07	3.5E-07	1.1E-06				15%	-8.3	-8.0	-9.4
hexahydro-1,3,5-trimethyl-1,3,5-triazine	203-612-8	108-74-7	108747	1488	Reach_754	1047	129	17.2	3.1E+02	8.1E+05	7.1E-03		8.91	3.5E-06	1.1E-07	3.5E-07				14%	-7.1	-8.0	-10.2
685-281-3	685-281-3	2624-17-1	2624171	5804	Reach_4630	1048	151	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.7	-8.0	-9.7
didodecyl 3,3'-thiodipropionate	204-614-1	123-28-4	123284	1767	Reach_1043	1049	515	155.2	8.7E-07	9.6E-07	6.2E+11			1.1E-06	1.1E-07	3.5E-07				24%	-8.2	-8.0	-8.6
N-ethyl-p-methoxy-α-methylphenethylamine	611-084-9	54041-17-7	54041177	3118	Reach_4348	1050	211	100.8	3.7E-04	1.6E+03	3.0E+01		14.5	3.5E-07	1.1E-07	3.5E-07				16%	-8.3	-8.0	-9.8
dimethyl succinate	203-419-9	106-65-0	106650	1441	Reach_676	1051	146	-95.3	5.8E+01	1.9E+05	2.5E+00			3.5E-06	3.5E-07	1.1E-06				14%	-8.3	-8.0	-10.0
tributyl citrate	201-071-2	77-94-1	77941	3745	Reach_191	1052	360	89.1	3.3E-05	1.2E+02	1.9E+03	9.92		3.5E-07	3.5E-08	1.1E-07				16%	-7.4	-8.0	-9.8
3-hydroxypropiononitrile	203-704-8	109-78-4	109784	1508	Reach_792	1053	71	-16.0	2.7E+00	2.0E+05	7.6E-02	13.9		1.1E-06	3.5E-07	1.1E-06				14%	-7.5	-8.0	-10.1
α-methylcinnamaldehyde	202-938-8	101-39-3	101393	1320	Reach_576	1054	146	2.6	3.3E+00	2.8E+02	2.3E+02			1.1E-06	1.1E-07	3.5E-07				15%	-8.3	-8.0	-9.6
methyl acetoacetate	203-299-8	105-45-3	105453	1413	Reach_640	1055	116	-31.2	1.7E+02	3.4E+04	2.0E-01	10.6		3.5E-06	3.5E-07	1.1E-06				14%	-8.2	-8.0	-9.9
dibutyl maleate	203-328-4	105-76-0	105760	183	Reach_650	1056	228	-28.2	7.1E-01	1.3E+02	1.4E+04			1.2E-06	3.5E-07	1.1E-06				16%	-8.3	-8.0	-9.7
hexadecyl methacrylate	219-672-3	2495-27-4	2495274	2410	Reach_1821	1057	311	81.6	3.5E-03	4.5E-03	4.4E+08			1.1E-06	1.1E-07	3.5E-07				23%	-7.9	-8.0	-9.5
3,3'-[(2,5-dimethyl-p-phenylene)bis[imino(1-acetyl-2-oxoethyle	226-107-4	5280-80-8	5280808	3076	Reach_2092	1058	917	349.8	3.5E-30	1.3E-09	8.5E+07	8.41	13.3	3.5E-08	1.1E-08	1.1E-08				21%	-8.5	-8.0	-9.3
m-(4,5-dihydro-3-methyl-5-oxo-1H-pyrazol-1-yl)benzenesulphc	204-303-0	119-17-5	119175	1686	Reach_976	1059	254	196.6	4.3E-09	1.1E+04	2.5E-01	0.7		1.1E-06	1.1E-07	3.5E-07				14%	-6.8	-8.0	-10.1
1-propoxypropan-2-ol	216-372-4	1569-01-3	1569013	2052	Reach_1693	1060	118	-33.5	1.8E+02	5.0E+04	3.1E+00	15.1		3.5E-07	1.1E-07	3.5E-07				16%	-8.3	-8.0	-9.6
(3R,4S,5R)-3,4,5-trihydroxycyclohex-1-enecarboxylic acid	700-265-9	2629-68-7	2629687	2463	Reach_4829	1061	247	2.7	1.2E+02	1.8E+01	3.5E+04			3.5E-07	3.5E-08	1.1E-07				15%	-6.9	-8.0	-9.9
4-chlorophenyl isocyanate	203-176-9	104-12-1	104121	1384	Reach_618	1062	154	-6.2	3.3E+01	8.9E+03	1.7E+03			3.5E-07	1.1E-07	3.5E-07				16%	-8.3	-8.0	-9.5
605-539-0	210-734-5	622-40-2	622402	762	Reach_1445	1063	131	36.1	1.9E+00	1.0E+06	4.8E-02									18%	-7.7	-8.0	-9.7
5-sulphoanthranilic acid	601-161-5	112110-16-4	112110164	1574	Reach_4080	1064	209	26.5	1.0E+00	3.0E+02	5.1E+00		14	1.1E-06	1.1E-07	3.5E-07				14%	-6.9	-8.0	-10.2
3,5,6-tri-O-.benzyl-1,2-O-isopropylidene-α-D-glucofuranose	242-160-6	18282-59-2	18282592	2175	Reach_2456	1065	226	37.2	7.2E+00	1.3E+01	1.5E+04			1.1E-07	1.1E-08	3.5E-08				20%	-7.4	-8.0	-9.5
1,8-naphthylenediamine	207-529-8	479-27-6	479276	646	Reach_1291	1066	158	109.7	5.0E-04	1.2E+03	2.2E+01		10	2.5E-09	1.1E-07	1.1E-06				23%	-7.8	-8.0	-9.0
1,3-dichloropropan-2-ol	202-491-9	96-23-1	96231	1049	Reach_456	1067	129	-23.6	4.1E+01	3.9E+04	6.0E+00	13.1		4.6E-07	3.5E-08	1.1E-07				15%	-8.3	-8.0	-9.8
sodium 1,2-diisobutoxycarbonylethanesulphonate	204-839-5	127-39-9	127399	5649	Reach_1097	1068	332	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.7	-8.0	-9.7
ethyl 2-chloroacetoacetate	210-180-4	609-15-4	609154	3319	Reach_1415	1069	165	-2.6	4.7E+01	2.6E+03	9.5E-01	7		3.5E-06	3.5E-07	1.1E-06				14%	-8.2	-8.0	-9.8
1,1'-(isopropylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)b	244-617-5	21850-44-2	21850442	2307	Reach_2511	1070	944	281.2	8.5E-13	5.1E-10	3.3E+11			1.1E-06	1.1E-07	3.5E-07				24%	-8.2	-8.0	-8.6
Ethyl N-([2-(chloromethyl)-1-methyl-1H-benzimidazol-5-yl]carb	233-897-4	10420-33-4	10420334	1387	Reach_2292	1071	188	-46.2	2.4E+01	8.9E+04	1.8E-01			3.5E-06	3.5E-07	1.1E-06				14%	-7.4	-8.0	-10.0
2-(11H-dibenzo[b,e]azepin-6-ylmethyl)-1H-isoindole-1,3(2H)-di	218-056-1	2043-57-4	2043574	2264	Reach_1748	1072	474	-15.8	3.9E+02	6.2E-04	4.3E+06			3.5E-07	1.1E-07	3.5E-07				14%	-7.5	-8.1	-10.0
616-309-4	204-516-9	122-03-2	122032	377	Reach_1025	1073	148	7.5	7.8E+00	1.7E+02	1.5E+03									18%	-7.7	-8.1	-9.7
morpholinium sulphamate	258-061-6	52636-67-6	52636676	5915	Reach_2786	1074	184	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.7	-8.1	-9.7
N,N'''-1,6-hexanediylbis[N'-cyanoguanidine]	240-032-4	15894-70-9	15894709	2065	Reach_2404	1075	250	197.7	3.5E-07	3.6E+03	7.6E-01	12.7	14.6	3.5E-07	1.1E-07	3.5E-07				16%	-7.0	-8.1	-9.9
choline hydrogen carbonate	201-137-0	78-73-9	78739	6039	Reach_206	1076	165	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.8	-8.1	-9.7
2,2'-dimorpholinyldiethyl ether	229-194-7	6425-39-4	6425394	3432	Reach_2184	1077	244	106.3	1.0E-02	2.8E+05	4.9E-02		7.46	1.1E-06	1.1E-07	3.5E-07				14%	-7.0	-8.1	-10.2
cyclohexyldimethylamine	202-715-5	98-94-2	98942	1080	Reach_525	1078	127	-39.2	3.3E+02	2.1E+03	2.0E+02		4	3.8E-08	3.5E-07	1.1E-06				22%	-8.3	-8.1	-9.6
triethyl citrate	201-070-7	77-93-0	77930	92	Reach_190	1079	276	22.7	2.6E-02	3.8E+03	2.1E+00	9.92		5.7E-07	3.5E-07	1.1E-06				15%	-7.8	-8.1	-10.0
oxybispropanediol	261-605-5	59113-36-9	59113369	3265	Reach_2834	1080	166	101.1	7.8E-05	1.0E+06	1.7E-03	13.8		1.1E-06	3.5E-07	1.1E-06				14%	-7.0	-8.1	-10.2
5-ethylidene-8,9,10-trinorborn-2-ene	240-347-7	16219-75-3	16219753	2083	Reach_2414	1081	120	-29.9	8.2E+02	3.0E+02	4.7E+03			1.1E-06	1.1E-07	3.5E-07				18%	-8.4	-8.1	-10.4
trioctyl benzene-1,2,4-tricarboxylate	201-877-4	89-04-3	89043	3967	Reach_337	1082	547	225.6	6.9E-10	2.0E-05	6.5E+11			1.1E-06	1.1E-07	3.5E-07				24%	-8.3	-8.1	-8.6
diethyl chloromalonate	229-014-7	6401-97-4	6401974	3422	Reach_2177	1083	173	104.9	3.3E-02	9.1E+02	1.6E+01			3.5E-07	3.5E-08	3.5E-07				16%	-8.3	-8.1	-9.7
tetrasodium hydrogen 2-phosphonatobutane-1,2,4-tricarboxyl	266-442-3	66669-53-2	66669532	5983	Reach_2883	1084	358	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.7	-8.1	-9.7
methylphosphonic acid	213-607-2	993-13-5	993135	4203	Reach_1627	1085	96	7.3	4.4E-02	4.6E+05	1.0E-01	2.6		1.1E-07	3.5E-08	1.1E-07				19%	-7.2	-8.1	-9.7
2-ethylhexane-1,3-diol	234-129-0	10545-99-0	10545990	6391	Reach_2296	1086	103	0.0												16%	-8.2	-8.1	-9.9
p-(1,1-dimethylpropyl)phenol	201-280-9	80-46-6	80466	936	Reach_263	1087	164	47.7	1.5E-01	7.1E+01	8.1E+03	10		2.6E-09	3.5E-07	1.1E-06				23%	-8.3	-8.1	-9.2
dodecyldimethylamine	203-943-8	112-18-5	112185	321	Reach_892	1088	213	22.5	2.1E+00	1.3E-01	2.8E+05		4	1.2E-07	3.5E-08	1.1E-07				23%	-8.4	-8.1	-10.6
618-465-9	618-465-9	9011-11-4	9011114	5587	Reach_4495	1089	222	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.8	-8.1	-9.7
cyclododecanone	212-595-6	830-13-7	830137	3840	Reach_1559	1090	182	29.8	6.7E-01	3.5E-01	1.2E+04			1.1E-06	1.1E-07	3.5E-07				18%	-8.4	-8.1	-10.3
bis(2-butoxyethyl) adipate	224-518-3	4394-85-8	4394858	2918	Reach_2031	1091	115	24.8	6.5E+00	2.6E+08	4.8E-02			1.1E-06	1.1E-07	3.5E-07				17%	-8.3	-8.1	-9.8
tetradecyl myristate	221-787-9	3234-85-3	3234853	2648	Reach_1936	1092	425	162.8	2.1E-06	1.3E-07	4.5E+12			1.1E-06	1.1E-07	3.5E-07				24%	-8.3	-8.1	-8.5
dimethyl 5-nitroisophthalate	616-149-5	74860-00-7	74860007	3648	Reach_4424	1093	352	253.8	6.4E-11	2.0E-01	1.9E+05			1.1E-06	1.1E-07	3.5E-07				14%	-8.3	-8.1	-10.0
methyl undec-10-enoate	203-910-8	111-81-9	111819	1558	Reach_872	1094	198	11.3	4.0E+00	1.1E+01	4.6E+04			3.5E-07	1.1E-07	3.5E-07				19%	-8.4	-8.1	-9.8
tetrahydrothiophene	203-728-9	110-01-0	110010	271	Reach_800	1095	88	-48.8	2.0E+03	8.4E+03	6.2E+01			2.2E-09	1.1E-07	3.5E-07				23%	-8.4	-8.1	-9.7
2,9-bis[4-(phenylazo)phenyl]anthra[2,1,9-def:6,5,10-d'e'f']diisc	221-264-5	3049-71-6	3049716	2600	Reach_1907	1096	751	349.8	9.8E-29	4.7E-11	2.6E+09		12.8	1.1E-07	3.5E-09	1.1E-08				19%	-8.5	-8.1	-9.6
sodium [N-[2-[bis(carboxymethyl)amino]ethyl]-N-(2-hydroxyetl	257-036-7	51181-50-1	51181501	5903	Reach_2770	1097	353	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.8	-8.1	-9.7
(6R-trans)-7-amino-3-methyl-8-oxo-5-thia-1-azabicyclo[4.2.0]o	210-765-4	623-03-0	623030	763	Reach_1447	1098	138	22.9	2.9E+00	2.5E+03	1.5E+02			5.3E-09	1.1E-08	3.5E-08				14%	-6.8	-8.1	-10.2
3,5-dichloronitrobenzene	225-139-6	4684-28-0	4684280	2958	Reach_2055	1099	289	158.0	5.7E-07	4.7E+03	1.5E+00			1.1E-06	1.1E-07	3.5E-07				23%	-8.4	-8.1	-9.3
silver docosanoate	211-792-4	696-29-7	696297	809	Reach_1512	1100	126	-61.0	5.5E+02	7.6E+00	3.2E+04									18%	-7.8	-8.1	-9.7
4-methylpentan-2-ol	203-551-7	108-11-2	108112	230	Reach_729	1101	102	-62.9	5.0E+02	1.6E+04	4.8E+01	16		4.0E-07	1.1E-06	3.5E-06				16%	-8.3	-8.1	-9.3
aziridine	205-793-9	151-56-4	151564	485	Reach_1208	1102	43	-59.7	3.1E+04	1.0E+06	5.2E-01		6	5.0E-07	3.5E-07	1.1E-06				15%	-8.3	-8.1	-9.2

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
2,4,6-triallyloxy-1,3,5-triazine	202-936-7	101-37-1	101371	1318	Reach_575	1103	249	124.1	2.8E-02	1.8E+02	1.9E+05		11.7	1.1E-06	3.5E-07	1.1E-06				14%	-7.5	-8.1	-10.0
D-N-(4-hydroxyphenyl)glycine	204-112-2	115-86-6	115866	9	Reach_946	1104	326	86.5	6.3E-05	2.3E+00	5.0E+04			6.1E-07	3.5E-08	1.1E-07				14%	-6.8	-8.1	-10.1
tetrasodium 7,7'-(carbonyldiimino)bis[4-hydroxy-3-[(6-sulphon	249-171-5	28706-25-4	28706254	5817	Reach_2622	1105	1061	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.8	-8.1	-9.7
Methyl 5-methyl-4-[(oxomethylene)sulfamoyl]thiophene-3-carl	618-297-6	897671-34-0	897671340	3985	Reach_4491	1106	261	151.7	1.7E-04	8.7E+02	1.0E+02			1.1E-06	1.1E-07	3.5E-07				14%	-7.3	-8.1	-10.0
1,1,1-trichloroethane	200-756-3	71-55-6	71556	822	Reach_104	1107	133	-72.0	1.5E+04	2.3E+03	4.8E+02			4.8E-08	1.1E-08	3.5E-08				23%	-8.5	-8.1	-10.6
3-hydroxy-2-naphthanilide	204-280-7	118-83-2	118832	1680	Reach_972	1108	226	52.1	2.9E+00	5.2E+01	2.6E+03			1.1E-06	3.5E-08	1.1E-07				18%	-7.4	-8.1	-9.8
7-hydroxynaphthalene-1-sulphonic acid	700-329-6	146763-69-1	146763691	1993	Reach_4863	1109	302	64.0	3.1E-03	3.1E+01	1.7E+03			1.1E-06	1.1E-07	3.5E-07				14%	-7.0	-8.1	-10.2
3-hydroxy-2-naphthoic acid	202-180-8	92-70-6	92706	4045	Reach_389	1110	188	141.0	8.3E-06	4.8E+02	2.6E+03	3		3.5E-06	1.1E-07	3.5E-07				14%	-7.4	-8.1	-10.1
isopropyl palmitate	205-571-1	142-91-6	142916	1957	Reach_1185	1111	299	72.0	2.7E-02	1.1E-02	1.4E+08			1.1E-06	1.1E-07	3.5E-07				23%	-8.0	-8.1	-10.0
oleic acid, compound with (Z)-N-octadec-9-enylpropane-1,3-di	248-704-9	27871-49-4	27871494	2521	Reach_2613	1112	104	-39.8	2.4E+02	3.4E+05	2.1E-01									18%	-7.8	-8.1	-9.8
3-methylbut-2-en-1-ol	209-141-4	556-82-1	556821	3176	Reach_1369	1113	86	-59.3	3.1E+02	4.9E+03	1.5E+01	15.5		3.5E-06	1.1E-06	3.5E-06				14%	-8.3	-8.1	-9.6
3-Bromo-1-(3-chloropyridin-2-yl)-1H-pyrazole-5-carboxylic acid	481-150-8	500011-86-9	500011869	2992	Reach_4012	1114	303	171.1	1.8E-05	1.6E+02	1.1E+02	3.43	13.5	1.1E-06	1.1E-07	3.5E-07				14%	-7.3	-8.1	-10.1
sodium 4-(methoxycarbonyl)phenolate	225-714-1	5026-62-0	5026620	5897	Reach_2070	1115	174	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.8	-8.1	-9.7
{5-chloro-2-[(cyclopropylmethyl)amino]phenyl}(phenyl)methar	201-332-0	81-19-6	81196	939	Reach_273	1116	230	45.7	1.2E+00	5.5E+00	1.8E+04	0	0	8.4E-08	1.1E-08	3.5E-08				23%	-7.6	-8.1	-9.2
suberonitrile	700-912-5	895525-76-5	895525765	3979	Reach_5025	1117	513	211.3	4.5E-08	3.6E-01	3.4E+05			1.1E-06	1.1E-07	3.5E-07				23%	-8.4	-8.1	-9.2
2,4,8,10-tetra(tert-butyl)-6-hydroxy-12H-dibenzo[d,g][1,3,2]dic	286-344-4	85209-91-2	85209912	6058	Reach_2984	1118	510	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.8	-8.1	-9.8
2-methyl-4-nitroimidazole	203-026-2	102-36-3	102363	1341	Reach_592	1119	188	24.2	9.5E+00	1.6E+02	7.6E+03			1.1E-07	1.1E-08	3.5E-08				14%	-6.9	-8.1	-10.2
benzyl salicylate	204-262-9	118-58-1	118581	1674	Reach_966	1120	228	115.5	2.4E-03	1.1E+02	2.0E+04	9.8		1.1E-06	1.1E-07	3.5E-07				16%	-8.1	-8.1	-9.9
tris[(2-hydroxyethyl)ammonium] citrate	244-599-9	21829-50-5	21829505	5774	Reach_2509	1121	375	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.8	-8.1	-9.8
O-acetylsalicylic acid	200-064-1	50-78-2	50782	666	Reach_9	1122	180	93.1	8.7E-03	2.3E+03	1.3E+01	3.5		1.1E-06	3.5E-07	1.1E-06				14%	-7.3	-8.1	-10.0
4-hydroxy-5-[[(p-tolyl)sulphonyl]amino]naphthalene-2,7-disulp	200-085-6	51-21-8	51218	668	Reach_13	1123	130	150.6	9.5E-06	1.0E+04	1.5E-01	7.8		2.2E-07	1.1E-07	3.5E-07				14%	-7.0	-8.1	-10.2
4-[(2,5-dichlorophenyl)azo]-3-hydroxy-N-phenylnaphthalene-2	227-930-1	6041-94-7	6041947	3310	Reach_2151	1124	436	276.0	1.3E-13	1.0E-02	3.8E+08	9.28		1.1E-07	3.5E-09	1.1E-08				24%	-8.1	-8.1	-8.7
calcium 4,5-dichloro-2-[[4,5-dihydro-3-methyl-5-oxo-1-(3-sulpl	213-234-5	931-36-2	931362	4059	Reach_1607	1125	110	62.5	2.5E-01	4.3E+03	4.4E+01									18%	-7.8	-8.1	-9.8
sodium diisobutyldithiophosphinate	236-419-2	13360-78-6	13360786	5667	Reach_2331	1126	232	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.8	-8.1	-9.8
pentafluoroethane	206-557-8	354-33-6	354336	2733	Reach_1246	1127	120	-162.1	9.5E+05	8.0E+01	3.5E+01			3.5E-08	1.1E-08	3.5E-08				23%	-8.5	-8.1	-10.9
2,2'-azobis[2-methylpropionamidine] dihydrochloride	221-070-0	2997-92-4	2997924	5829	Reach_1895	1128	271	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.8	-8.1	-9.8
zinc diricinoleate	235-911-4	13040-19-2	13040192	5659	Reach_2319	1129	660	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.8	-8.1	-9.8
[[4-[[4-(anilino)phenyl][4-(phenylimino)-2,5-cyclohexadien-1-yl	215-385-2	1324-76-1	1324761	1858	Reach_1677	1130	596	349.8	7.9E-22	4.0E-07	3.2E+06	-1.37	10.6	3.5E-07	3.5E-08	1.1E-07				16%	-7.7	-8.1	-9.9
N,N-dimethylaniline	261-619-1	59130-69-7	59130697	3268	Reach_2835	1131	369	117.2	1.4E-04	3.2E-05	4.1E+10		0	1.1E-06	1.1E-07	3.5E-07				23%	-8.3	-8.1	-9.2
maleic acid	203-742-5	110-16-7	110167	275	Reach_806	1132	116	84.1	1.3E-09	5.5E+04	1.1E+00	3		4.7E-06	3.5E-07	1.1E-06				14%	-6.9	-8.1	-10.1
p-(dimethoxymethyl)anisole	218-577-4	2186-92-7	2186927	2308	Reach_1770	1133	182	22.9	6.5E+00	1.9E+03	3.3E+01			1.1E-06	1.1E-07	3.5E-07				14%	-8.3	-8.1	-9.8
bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate	258-207-9	52829-07-9	52829079	3077	Reach_2788	1134	481	210.7	5.0E-08	3.3E-01	3.2E+06		4.1	1.1E-06	1.1E-07	3.5E-07				20%	-7.7	-8.1	-9.5
1-chloro-2,5-dimethoxybenzene	218-267-9	2100-42-7	2100427	2282	Reach_1758	1135	173	24.8	1.4E+01	5.0E+02	6.3E+02			1.1E-06	1.1E-07	3.5E-07				15%	-8.4	-8.1	-9.6
6-methoxy-m-toluidine	204-419-1	120-71-8	120718	1718	Reach_1000	1136	137	45.8	4.2E+00	8.3E+03	5.0E+01		9.4	1.1E-06	3.5E-07	1.1E-06				14%	-7.5	-8.1	-10.1
1,1,3,3-tetramethylbutylamine	203-491-1	107-45-9	107459	220	Reach_708	1137	129	-20.0	9.7E+02	1.4E+00	3.8E+02		4	6.6E-09	1.1E-07	3.5E-07				24%	-8.4	-8.1	-10.9
benzyl acetate	205-399-7	140-11-4	140114	448	Reach_1147	1138	150	-0.5	2.5E+01	2.9E+03	1.2E+02			6.7E-07	1.1E-07	3.5E-07				15%	-8.4	-8.1	-9.6
!4-methylmorpholine 4-oxide! !monohydrate!	231-391-8	7529-22-8	7529228	3663	Reach_2258	1139	117	125.1	2.4E-03	4.0E+07	7.6E-02		9.63	1.1E-06	1.1E-07	3.5E-07				14%	-6.9	-8.1	-10.2
6,6',6''-(1,3,5-triazine-2,4,6-triyltriimino)trihexanoic acid	279-505-5	80584-91-4	80584914	3795	Reach_2959	1140	469	301.0	3.6E-14	2.0E-06	2.1E+04	4.22	8.08	1.1E-06	1.1E-07	3.5E-07				14%	-7.5	-8.1	-10.0
bis(piperidinothiocarbonyl) hexasulphide	213-537-2	971-15-3	971153	4161	Reach_1621	1141	449	242.4	3.8E-10	8.9E-03	2.7E+04		15.2	3.5E-07	1.1E-07	3.5E-07				16%	-7.7	-8.1	-9.9
(1S,3R,7S,8S,8aR)-8-{2-[(2R,4R)-4-hydroxy-6-oxotetrahydro-2H	220-374-0	2743-38-6	2743386	2506	Reach_1862	1142	358	207.9	3.4E-08	7.1E+03	7.8E+03	1.07		1.1E-06	3.5E-07	1.1E-06				19%	-7.4	-8.1	-9.6
617-251-2	250-439-9	31027-31-3	31027313	2618	Reach_2651	1143	161	-7.2	3.3E+01	1.2E+03	1.1E+04			3.5E-07	1.1E-07	3.5E-07				14%	-7.1	-8.1	-10.2
isoquinoline	204-341-8	119-65-3	119653	356	Reach_984	1144	129	37.6	4.9E+00	2.0E+03	1.4E+02		9	3.4E-07	3.5E-08	1.1E-07				16%	-7.9	-8.1	-10.0
2,2,6,6-tetramethyl-4-piperidylamine	202-678-5	98-53-3	98533	4186	Reach_510	1145	154	8.4	2.3E+01	3.4E+02	8.1E+02			1.1E-06	3.5E-07	1.1E-06				14%	-8.4	-8.1	-10.0
3-chloropropyl(dimethyl)amine	239-349-0	15307-93-4	15307934	2029	Reach_2383	1146	238	99.7	1.0E-02	2.9E+00	3.8E+04			1.1E-06	3.5E-08	1.1E-07				16%	-8.4	-8.1	-9.5
(Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine	203-749-3	110-25-8	110258	1515	Reach_809	1147	354	196.1	2.3E-07	6.0E-02	6.8E+06	3.3		1.1E-06	1.1E-07	3.5E-07				15%	-7.4	-8.1	-10.0
2-ethyl-2-[[(1-oxoallyl)oxy]methyl]-1,3-propanediyl diacrylate	239-701-3	15625-89-5	15625895	2046	Reach_2391	1148	296	27.2	7.5E-02	7.1E+01	7.2E+02			3.5E-06	3.5E-07	1.1E-06				14%	-8.4	-8.1	-10.0
di(succinimido) carbonate	604-349-5	143382-03-0	143382030	1964	Reach_4149	1149	211	162.2	6.7E-05	4.6E+03	4.6E-01			1.1E-06	1.1E-07	3.5E-07				14%	-7.0	-8.1	-10.2
1,3-diphenylguanidine	203-002-1	102-06-7	102067	1335	Reach_588	1150	211	120.1	5.3E-04	1.0E+02	7.8E+02		3.9	3.5E-06	1.1E-07	3.5E-07				14%	-7.7	-8.1	-10.1
605-014-6	605-014-6	1555-62-0	1555620	2042	Reach_4166	1151	291	146.6	2.7E-05	2.4E+01	3.0E+04		9.5	1.1E-06	1.1E-07	3.5E-07				14%	-7.6	-8.1	-10.1
2-imidazolidone	200-074-6	50-98-6	50986	5902	Reach_11	1152	202	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				16%	-8.1	-8.1	-10.0
dimethyl 2-nitroterephthalate	226-134-1	5292-45-5	5292455	680	Reach_2094	1153	239	76.9	2.5E-02	1.6E+02	3.0E+01			7.5E-07	1.1E-07	3.5E-07				15%	-8.4	-8.1	-10.1
betaine	203-490-6	107-43-7	107437	1462	Reach_707	1154	117	160.3	7.1E-05	1.0E+06	1.2E-03	1.9		3.5E-06	3.5E-07	1.1E-06				14%	-6.8	-8.1	-10.2
3,4-diaminobenzenesulphonic acid	239-138-3	15086-94-9	15086949	2013	Reach_2376	1155	648	284.2	1.9E-15	5.3E-05	8.1E+06	6.14		1.1E-06	1.1E-08	3.5E-08				14%	-7.0	-8.1	-10.2
2,4,6-tris(dimethylaminomethyl)phenol	202-013-9	90-72-2	90722	4003	Reach_366	1156	265	133.8	2.1E-04	5.8E+04	5.9E+00	11.8	5.37	3.5E-06	3.5E-07	1.1E-06				14%	-7.2	-8.1	-10.2
pin-2(3)-ene	201-291-9	80-56-8	80568	937	Reach_267	1157	136	-13.6	5.4E+02	2.8E+01	1.9E+04			9.7E-08	3.5E-08	1.1E-07				23%	-8.4	-8.1	-10.7
disodium 2-hydroxyethyliminodi(acetate)	617-500-5	83905-01-5	83905015	957	Reach_4465	1158	749	349.8	3.5E-22	7.4E-01	1.7E+03									18%	-7.8	-8.1	-9.8
l-Glutamic acid, N-coco acyl derivs., monosodium salts	269-087-2	68187-32-6	68187326	5994	Reach_2900	1159	337	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.8	-8.1	-9.8
2-nitropropane	201-209-1	79-46-9	79469	921	Reach_247	1160	89	-37.9	2.1E+03	1.6E+04	7.4E+00	8.2		2.2E-09	3.5E-07	1.1E-06				23%	-8.4	-8.1	-9.5
[7(S)-(1α,.2β,4β,5α,7β)]-3-oxa-9-azatricyclo[3.3.1.02,4]non-7-y	241-475-6	17462-58-7	17462587	2140	Reach_2433	1161	137	-55.7	1.6E+03	1.7E+03	3.5E+01			3.5E-06	3.5E-07	1.1E-06				14%	-7.0	-8.1	-10.3
4-chlorotoluene	202-809-6	100-00-5	100005	119	Reach_546	1162	158	48.8	1.5E+00	4.0E+02	2.9E+02			2.2E-09	1.1E-07	3.5E-07				23%	-8.5	-8.1	-10.4
ethylenediamine-N,N'-bis((2-hydroxyphenyl)acetic acid)	225-195-1	4708-04-7	4708047	1271	Reach_2057	1163	161	-34.8	1.9E+02	8.5E+03	7.2E+00			1.1E-06	3.5E-07	1.1E-06				14%	-6.9	-8.1	-10.3
calcium diethyl bis[[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphen	260-353-3	56718-70-8	56718708	3210	Reach_2820	1164	208	67.5	1.8E-01	1.3E+03	7.8E+01									18%	-7.8	-8.1	-9.8
607-145-4	607-578-9	25157-64-6	25157646	2418	Reach_4244	1165	282	349.8	2.9E-19	1.0E+06	2.3E-03			1.1E-06	1.1E-07	3.5E-07				19%	-8.4	-8.1	-9.5
618-837-0	618-837-0	92339-11-2	92339112	6408	Reach_4501	1166	1550	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.8	-8.1	-9.8
triphenylphosphine oxide	614-050-1	67330-25-0	67330250	3489	Reach_4394	1167	337	130.3	3.0E-04	2.7E-01	8.3E+06			1.1E-06	1.1E-07	3.5E-07				23%	-8.0	-8.1	-9.2
2,6-dimethyloct-7-en-2-ol	242-362-4	18479-58-8	18479588	2192	Reach_2463	1168	156	-13.1	1.7E+01	7.4E+02	3.0E+03	16		1.1E-06	1.1E-07	3.5E-07				15%	-8.4	-8.1	-9.6
dapsone	201-248-4	80-08-0	80080	3787	Reach_256	1169	248	182.9	3.6E-06	2.1E+03	5.9E+00		12.2	1.1E-06	3.5E-07	1.1E-06				14%	-7.2	-8.2	-10.1
5-(methoxymethyl)pyridine-2,3-dicarboxylic acid	203-801-5	110-76-9	110769	1530	Reach_827	1170	89	-40.4	3.5E+03	2.1E+05	3.8E-01		4.5	1.1E-06	1.1E-07	3.5E-07				14%	-7.1	-8.2	-10.3
3-Bromo-5-chlorophenol	206-337-1	328-84-7	328847	2665	Reach_1235	1171	215	1.5	1.8E+02	8.3E+00	1.7E+04			1.1E-07	1.1E-08	3.5E-08				15%	-8.4	-8.2	-10.1
8,9,10,11-tetrachloro-12H-phthaloperin-12-one	244-007-9	20749-68-2	20749682	2272	Reach_2497	1172	408	230.9	2.3E-09	3.7E-04	6.2E+05		6.8	1.1E-08	3.5E-09	3.5E-09				23%	-7.9	-8.2	-9.1
3-amino-5-chloro-2-hydroxybenzenesulphonic acid	228-169-8	6153-06-6	6153066	1280	Reach_2155	1173	96	-21.5	6.7E+01	4.5E+04	7.8E+00	15.5		3.5E-06	1.1E-06	3.5E-06				14%	-6.9	-8.2	-10.3
butyric acid	203-532-3	107-92-6	107926	224	Reach_719	1174	88	3.0	2.8E+02	1.1E+05	1.2E+01	4.9		4.1E-06	3.5E-07	1.1E-06				14%	-7.7	-8.2	-10.1
O,O-diethyl phosphorochloridothioate	246-309-6	24549-06-2	24549062	2397	Reach_2549	1175	135	40.1	9.9E+00	1.3E+03	4.6E+02			1.1E-06	1.1E-07	3.5E-07				17%	-8.4	-8.2	-9.7
3-chloro-o-toluidine	252-276-9	34893-92-0	34893920	2717	Reach_2684	1176	188	24.2	1.5E+01	1.6E+02	7.6E+03			1.1E-07	1.1E-08	3.5E-08				14%	-7.6	-8.2	-10.1
2,2',6,6'-tetrabromo-4,4'-isopropylidenediphenol	201-236-9	79-94-7	79947	929	Reach_252	1177	544	206.2	4.6E-09	1.9E-03	1.6E+07	7.73		4.1E-08	3.5E-07	1.1E-06				23%	-7.3	-8.2	-8.5

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
3,5-dinitrobenzoic acid	700-313-9	21134-38-3	21134383	2283	Reach_4855	1178	206	10.1	2.8E+01		1.7E-01			3.5E-06	3.5E-07	1.1E-06				14%	-7.2	-8.2	-10.3
hyoscine	605-999-2	18361-03-0	18361030	2185	Reach_4188	1179	230	173.4	1.3E-05	9.2E+03	4.3E+01	2.8		3.5E-06	3.5E-07	1.1E-06				14%	-7.1	-8.2	-10.3
2-butyl-2-ethylpropanediol	204-111-7	115-84-4	115844	1639	Reach_945	1180	160	42.7	8.1E-02	3.2E+04	1.3E+02	15.3		1.1E-06	3.5E-07	1.1E-06				14%	-7.7	-8.2	-10.0
5,5-dimethylhydantoin	201-051-3	77-71-4	77714	883	Reach_181	1181	128	150.3	1.8E-04	1.7E+04	5.4E-01	9.1	14	1.8E-07	3.5E-07	1.1E-06				17%	-7.4	-8.2	-9.9
chlorhexidine	200-238-7	55-56-1	55561	3175	Reach_23	1182	505	303.1	1.6E-12	1.4E-02	7.1E+04		2.71	1.1E-07	1.1E-08	3.5E-08				20%	-7.5	-8.2	-9.6
6,6'-di-tert-butyl-2,2'-methylenedi-p-cresol	204-327-1	119-47-1	119471	1692	Reach_978	1183	341	186.8	3.3E-07	1.9E-02	9.3E+07	10.5		1.1E-06	1.1E-07	3.5E-07				22%	-7.7	-8.2	-9.0
methylpentynol	201-055-5	77-75-8	77758	885	Reach_183	1184	98	-22.6	7.5E+02	8.0E+04	8.7E+00	13.6		2.2E-08	3.5E-07	1.1E-06				22%	-8.4	-8.2	-9.3
3-(dimethylamino)-1-(thiophen-2-yl)propan-1-ol	207-185-9	447-61-0	447610	2932	Reach_1277	1185	174	-6.2	9.0E+01	9.1E+02	4.7E+02			1.1E-06	3.5E-07	1.1E-06				14%	-7.2	-8.2	-10.3
bis(2-dimethylaminoethyl)(methyl)amine	221-201-1	3030-47-5	3030475	2590	Reach_1898	1186	173	10.5	3.9E+01	2.0E+05	2.7E-01		4.79	1.1E-06	1.1E-07	3.5E-07				14%	-8.4	-8.2	-10.2
sodium 3-[(1,5-dihydroxy-2-naphthyl)azo]-4-hydroxybenzenesu	229-114-0	6413-10-1	6413101	1284	Reach_2180	1187	174	25.3	1.8E+01	5.2E+04	2.0E+01									18%	-7.9	-8.2	-9.8
tamoxifen	234-118-0	10540-29-1	10540291	174	Reach_2294	1188	372	180.9	4.6E-06	8.6E-03	2.0E+06		6	1.6E-08	3.5E-08	1.1E-07				23%	-7.9	-8.2	-9.0
3,3',5,5'-tetramethylbiphenyl-2,2'-diol	628-771-4	23357-46-2	23357462	2349	Reach_4589	1189	147	48.0	2.7E+00	7.5E+02	2.6E+02			3.5E-07	3.5E-08	1.1E-07				19%	-7.7	-8.2	-9.8
N,N'-di-sec-butyl-p-phenylenediamine	202-992-2	101-96-2	101962	1331	Reach_585	1190	220	76.3	2.1E-01	1.2E+01	3.2E+03		7.7	3.5E-07	3.5E-08	1.1E-07				16%	-8.4	-8.2	-9.7
3,5-dimethylpyrazole	200-657-5	67-51-6	67516	3494	Reach_82	1191	96	27.6	2.8E+00	7.9E+03	1.4E+01		9.8	3.5E-07	3.5E-08	1.1E-07				16%	-7.2	-8.2	-10.1
bis(2-ethylhexyl) maleate	205-524-5	142-16-5	142165	1948	Reach_1172	1192	341	28.9	2.6E-01	9.8E-03	8.7E+07			3.5E-07	3.5E-08	1.1E-07				23%	-8.2	-8.2	-10.2
sulisobenzone	235-469-2	12237-63-7	12237637	5628	Reach_2309	1193	568	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				21%	-7.3	-8.2	-9.4
Methyl dec-9-enoate	231-658-9	7680-73-1	7680731	6032	Reach_2268	1194	130	0.0												19%	-8.5	-8.2	-9.9
Benzyl [(3aS,4R,6S,6aR)-6-hydroxy-2,2-dimethyltetrahydro-3aH	700-224-5	1647-12-7	1647127	2093	Reach_4810	1195	128	-57.4	1.2E+03	4.5E+03	1.3E+02			3.5E-06	3.5E-07	1.1E-06				15%	-7.4	-8.2	-10.0
1-(3-sulphonatopropyl)pyridinium	239-491-3	15471-17-7	15471177	2039	Reach_2389	1196	201	119.0	4.2E-05	4.9E+03	4.0E-04	0.23		3.5E-07	3.5E-08	1.1E-07				16%	-7.2	-8.2	-10.1
butan-2-one O,O',O''-(methylsilylidyne)trioxime	245-366-4	22984-54-9	22984549	2341	Reach_2525	1197	301	3.2	5.5E-02	7.0E-01	6.8E+09			3.5E-07	1.1E-07	3.5E-07				24%	-8.1	-8.2	-8.8
3-methyl-2-butenal	203-527-6	107-86-8	107868	1469	Reach_716	1198	84	-76.8	1.1E+03	1.2E+04	1.4E+01			3.5E-06	1.1E-06	3.5E-06				14%	-8.4	-8.2	-9.7
methacrylamide	201-202-3	79-39-0	79390	3775	Reach_244	1199	85	33.3	3.9E+00	2.8E+05	5.5E-01	15.1	14.4	3.5E-06	3.5E-07	1.1E-06				14%	-7.7	-8.2	-10.3
bis(2-(2-methoxyethoxy)ethyl) ether	205-594-7	143-24-8	143248	28	Reach_1191	1200	222	40.4	1.2E+00	2.2E+05	9.3E-02			8.2E-07	1.1E-07	1.1E-06				15%	-7.7	-8.2	-10.2
TCA (reach)	211-479-2	650-51-1	650511	1230	Reach_1486	1201	185	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.9	-8.2	-9.8
fenofibrate	618-126-5	88196-70-7	88196707	3950	Reach_4487	1202	151	34.4	7.6E+00	6.1E+03	3.7E+01			1.1E-06	1.1E-07	3.5E-07				22%	-8.2	-8.2	-9.4
627-082-6	627-082-6	89878-14-8	89878148	3989	Reach_4583	1203	147	3.6	5.0E+01		7.6E+02		8.8	3.5E-07	3.5E-08	1.1E-07				16%	-8.5	-8.2	-9.7
benzoxonium chloride	243-008-1	19379-90-9	19379909	5758	Reach_2478	1204	400	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.9	-8.2	-9.8
isopropyl oleate	203-935-4	112-11-8	112118	1575	Reach_888	1205	325	88.6	1.5E-03	2.3E-03	8.3E+08			1.1E-06	1.1E-07	3.5E-07				23%	-8.0	-8.2	-9.5
2-(bromomethyl)-2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxolan	262-103-9	60207-89-8	60207898	3308	Reach_2846	1206	354	129.9	6.2E-04	3.8E-01	3.3E+05			3.5E-07	3.5E-08	1.1E-07				20%	-8.3	-8.2	-9.7
3-(trimethoxysilyl)propyl isocyanate	239-415-9	15396-00-6	15396006	2033	Reach_2387	1207	205	32.9	1.2E+01		1.8E+00			1.1E-06	1.1E-07	1.1E-06				14%	-8.1	-8.2	-10.2
Ethyl 3-amino-4-[2-(phthalimido)ethoxy]crotonate	238-339-3	14367-46-5	14367465	1969	Reach_2364	1208	193	47.3	7.9E-01	2.4E+03	6.2E+02		4.1	3.5E-07	1.1E-07	3.5E-07				14%	-7.1	-8.2	-10.3
salbutamol	242-424-0	18559-94-9	18559949	2198	Reach_2465	1209	239	145.8	1.2E-06	1.6E+04	4.4E+00	10.1	5.06	1.1E-06	1.1E-07	3.5E-07				14%	-7.1	-8.2	-10.3
605-637-3	222-818-9	3621-82-7	3621827	2762	Reach_1976	1210	188	66.3	6.4E-01	9.0E+01	1.0E+03			1.1E-07	1.1E-08	3.5E-08				14%	-7.1	-8.2	-10.3
601-262-4	601-262-4	1135-22-4	1135224	1622	Reach_4082	1211	218	102.6	4.7E-04	8.7E+03	9.5E+00	16		1.1E-06	1.1E-07	3.5E-07				14%	-7.2	-8.2	-10.2
paracetamol	281-339-3	83929-47-9	83929479	3853	Reach_2968	1212	369	222.4	8.3E-09	1.1E-01	1.2E+03	12.7	0	3.5E-06	1.1E-07	3.5E-07				23%	-7.5	-8.2	-9.1
4-(3-methyl-5-oxo-2-pyrazolin-1-yl)benzenesulphonic acid	203-607-0	108-69-0	108690	244	Reach_753	1213	121	29.1	1.8E+01	5.9E+02	1.5E+02			2.8E-07	3.5E-08	1.1E-07				14%	-7.0	-8.2	-10.3
4-morpholinecarbaldehyde	205-466-0	141-18-4	141184	1934	Reach_1159	1214	346	32.6	4.8E-03	1.6E+01	6.0E+03			3.5E-07	3.5E-08	1.1E-07				14%	-6.9	-8.2	-10.3
[hexane-1,6-diylbis[nitrilobis(methylene)]]tetrakisphosphonic a	254-135-7	38820-59-6	38820596	5871	Reach_2718	1215	721	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.9	-8.2	-9.9
1,3-dihydro-5-methoxy-2H-benzimidazole-2-thione	253-326-2	37052-78-1	37052781	2789	Reach_2709	1216	180	143.5	9.0E-05	8.7E+02	1.0E+02	11.4	15.7	1.1E-06	1.1E-07	3.5E-07				14%	-7.4	-8.2	-10.2
604-848-8	700-822-6	1026785-65-8	1026785658	1350	Reach_5001	1217	547	243.1	3.4E-10	4.4E-02	1.4E+06			1.1E-06	1.1E-07	3.5E-07				14%	-7.5	-8.2	-10.3
618-706-8	202-445-8	95-73-8	95738	4131	Reach_438	1218	161	3.6	4.6E+01	6.1E+01	6.8E+03			1.1E-07	1.1E-08	3.5E-08				19%	-8.1	-8.2	-9.9
4-hydroxynaphthalene-1-sulphonic acid	680-587-3	144163-97-3	144163973	1972	Reach_4626	1219	280	153.0	3.5E-05	1.1E+02	9.5E+01			1.1E-06	1.1E-07	3.5E-07				14%	-7.0	-8.2	-10.3
6-hydroxynaphthalene-2-sulphonic acid	646-413-5	144689-24-7	144689247	1977	Reach_4613	1220	447	325.4	2.3E-19	4.2E-03	4.3E+03	2.4		3.5E-07	1.1E-08	3.5E-08				14%	-7.0	-8.2	-10.3
N-(4-chloro-2,5-dimethoxyphenyl)-3-hydroxy-4-[[2-methoxy-5-	226-103-2	5280-68-2	5280682	3074	Reach_2090	1221	611	349.8	9.5E-22	1.9E-04	2.1E+08	9.41	12.8	3.5E-07	1.1E-08	3.5E-08				16%	-7.8	-8.2	-10.1
1,2,3,6-tetrahydro-4-methylphthalic anhydride	222-323-8	3425-89-6	3425896	2699	Reach_1960	1222	166	15.9	3.2E+00	8.1E+03	3.2E+02			3.5E-06	3.5E-07	1.1E-06				14%	-8.4	-8.2	-10.1
(Z)-pent-2-enenitrile	229-353-0	6485-55-8	6485558	3445	Reach_2190	1223	115	0.9	6.3E+02	5.0E+03	1.9E+00			3.5E-06	3.5E-07	1.1E-06				16%	-8.5	-8.2	-9.6
2-mercaptoethanol	200-464-6	60-24-2	60242	749	Reach_56	1224	78	-45.6	1.1E+02	1.0E+05	6.3E-01	9.7		4.2E-06	1.1E-06	3.5E-06				14%	-8.4	-8.2	-10.1
bis(4-(1,1,3,3-tetramethylbutyl)phenyl)amine	239-816-9	15721-78-5	15721785	2055	Reach_2395	1225	394	165.2	6.7E-06	1.7E-05	6.6E+10		13.2	1.1E-06	3.5E-08	1.1E-07				15%	-7.2	-8.2	-9.9
heptanal	203-898-4	111-71-7	111717	1554	Reach_867	1226	114	-43.0	4.7E+02	1.6E+03	1.9E+02			3.5E-07	1.1E-07	3.5E-07				17%	-8.5	-8.2	-9.8
6-methyl-1,3,5-triazine-2,4-diyldiamine	267-135-7	67801-15-4	67801154	3500	Reach_2889	1227	206	44.5	1.9E+00	3.0E+00	2.6E+04		0	1.1E-06	3.5E-07	1.1E-06				19%	-7.4	-8.2	-9.8
4-(methylsulfonyl)-2-nitrobenzoic acid	601-017-1	110964-79-9	110964799	1534	Reach_4077	1228	245	174.5	1.1E-05	2.9E+02	8.3E-01	1.57		3.5E-06	1.1E-07	3.5E-07				14%	-7.0	-8.2	-10.4
2-[2-(Piperazin-1-yl)ethoxy]ethanol	224-970-1	4584-46-7	4584467	5891	Reach_2049	1229	144	0.0												14%	-7.2	-8.2	-10.3
azacyclonol	608-748-5	324763-46-4	324763464	2653	Reach_4281	1230	462	305.5	1.7E-14	9.7E-03	4.1E+06			1.1E-06	1.1E-07	3.5E-07				15%	-7.4	-8.2	-10.0
ethyltriphenylfosfonium bromide	214-447-6	1129-42-6	1129426	1612	Reach_1663	1231	172	155.0	1.9E-04	3.3E+05	1.5E-02			3.5E-06	1.1E-06	3.5E-06				19%	-8.5	-8.2	-9.7
pivaloyl chloride	221-921-6	3282-30-2	3282302	601	Reach_1941	1232	121	-48.0	4.3E+03	2.9E+03	7.8E+00			3.2E-08	3.5E-07	1.1E-06				23%	-8.5	-8.2	-10.3
N-(2,5-dimethoxyphenyl)acetamide	203-955-3	112-29-8	112298	324	Reach_895	1233	221	4.7	9.5E+00	1.7E-01	4.0E+05			5.0E-07	3.5E-08	1.1E-07				14%	-7.3	-8.2	-10.3
ethyl (S)-2-hydroxypropionate	211-694-1	687-47-8	687478	3526	Reach_1503	1234	118	-27.8	1.4E+02	3.7E+04	6.6E-01	12.6		3.5E-06	3.5E-07	1.1E-06				14%	-8.4	-8.2	-10.0
2,9-dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione	221-424-4	3089-17-6	3089176	2615	Reach_1916	1235	381	253.7	6.0E-13	5.1E-03	9.3E+04	10.2	14.6	1.1E-07	1.1E-08	3.5E-08				19%	-7.9	-8.2	-9.8
benzoin	204-331-3	119-53-9	119539	1694	Reach_979	1236	212	106.6	7.7E-05	1.1E+03	6.9E+01	12.3		1.1E-06	1.1E-07	3.5E-07				14%	-7.4	-8.2	-10.2
pentane-2,4-dione	204-634-0	123-54-6	123546	395	Reach_1052	1237	100	-29.4	1.2E+03	4.6E+05	1.1E+00	8.9		4.8E-06	3.5E-07	1.1E-06				14%	-8.4	-8.2	-10.1
anthranilic acid	204-287-5	118-92-3	118923	1683	Reach_974	1238	137	94.1	1.0E-02	1.4E+04	2.3E+01	5.08	11.7	1.1E-06	1.1E-07	3.5E-07				14%	-7.3	-8.2	-10.2
4-amino-2,5-dimethoxy-N-methylbenzenesulphonamide	256-435-3	49701-24-8	49701248	2986	Reach_2763	1239	246	154.6	8.3E-05	2.6E+04	1.2E+00	10.5	12.3	1.1E-06	1.1E-07	3.5E-07				14%	-7.0	-8.2	-10.3
dimethyl(tetradecyl)amine	204-002-4	112-75-4	112754	1601	Reach_922	1240	241	43.2	2.7E-01	1.4E-02	2.6E+06		3.9	1.1E-06	1.1E-07	3.5E-07				22%	-8.4	-8.2	-11.0
trimethyl orthoformate	205-745-7	149-73-5	149735	480	Reach_1201	1241	106	-75.5	4.9E+03	6.0E+04	9.3E-01			1.2E-06	1.1E-07	3.5E-07				15%	-8.5	-8.2	-9.8
4,4'-oxydi(benzenesulphonohydrazide)	201-286-1	80-51-3	80513	3792	Reach_264	1242	358	236.9	8.9E-10	1.9E+04	1.2E+00		5.75	1.1E-06	1.1E-07	3.5E-07				14%	-7.1	-8.2	-10.3
methanesulphonyl chloride	204-706-1	124-63-0	124630	404	Reach_1079	1243	115	-7.5	3.1E+02	7.1E+04	1.9E+01			7.8E-07	1.1E-06	3.5E-06				15%	-8.5	-8.2	-9.8
isobutyl acetate	203-745-1	110-19-0	110190	277	Reach_808	1244	116	-68.4	2.4E+03	1.1E+04	5.9E+01			9.1E-07	3.5E-07	1.1E-06				15%	-8.5	-8.2	-9.9
cyclopentanone	204-435-9	120-92-3	120923	364	Reach_1005	1245	84	-40.6	1.6E+03	4.4E+04	4.3E+00			9.4E-07	3.5E-07	1.1E-06				15%	-8.5	-8.2	-9.6
2-[(1R,4R,4aS,8aR)-4,7-dimethyl-1,2,3,4,4a,5,6,8a-octahydrona	609-904-5	41263-74-5	41263745	2874	Reach_4315	1246	196	139.3	8.0E-04	1.5E+03	7.9E+01	4.06		3.5E-06	3.5E-08	1.1E-07				15%	-7.6	-8.2	-10.1
2-hydroxy-2-methylpropiophenone	231-272-0	7473-98-5	7473985	3642	Reach_2253	1247	164	54.5	9.8E-02	8.6E+03	1.2E+01	13.4		1.1E-06	1.1E-07	3.5E-07				14%	-7.9	-8.2	-10.2
cyclododecane	206-033-9	294-62-2	294622	587	Reach_1225	1248	168	-18.5	3.1E+00	1.4E-01	1.3E+06			7.2E-09	1.1E-07	3.5E-07				24%	-8.5	-8.2	-10.7
4-amino-2,5-dimethoxy-N-phenylbenzenesulphonamide	257-821-4	52298-44-9	52298449	3056	Reach_2779	1249	308	196.0	4.6E-07	1.8E+02	7.6E+01	10.5	12.3	1.1E-06	1.1E-07	3.5E-07				14%	-7.4	-8.2	-10.2
2-(propyloxy)ethanol	220-548-6	2807-30-9	2807309	2522	Reach_1870	1250	104	-32.1	1.8E+02	1.9E+05	1.2E+00	15		1.1E-06	3.5E-07	1.1E-06				14%	-8.5	-8.2	-10.1
1,3-dioxolane	211-463-5	646-06-0	646060	780	Reach_1482	1251	74	-75.3	1.4E+04	9.0E+05	4.9E-01			4.1E-06	1.1E-07	3.5E-07				14%	-8.5	-8.2	-10.0
decane	204-686-4	124-18-5	124185	402	Reach_1072	1252	142	-44.1	2.3E+02	4.0E-01	1.8E+05			3.1E-07	3.5E-08	1.1E-07				23%	-8.5	-8.2	-11.0

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
N-(trimethylsilyl)imidazole	610-491-9	500011-92-7	500011927	2993	Reach_4330	1253	331	161.1	7.9E-05	2.3E+01	3.1E+02		13.6	1.1E-06	1.1E-07	3.5E-07				16%	-8.5	-8.2	-9.7
p-benzoquinone	203-405-2	106-51-4	106514	197	Reach_673	1254	108	23.7	3.4E+00	1.2E+04	1.8E+00			1.9E-06	3.5E-07	1.1E-06				14%	-8.4	-8.2	-10.2
phthalic acid	224-427-9	4355-11-7	4355117	1268	Reach_2029	1255	200	133.2	8.8E-04	2.2E+03	9.3E+01	3.6		1.1E-06	3.5E-07	1.1E-06				14%	-7.4	-8.2	-10.2
616-206-4	600-709-0	106006-84-2	106006842	1424	Reach_4071	1256	225	175.6	9.5E-06	5.3E+01	4.8E+01	15.1	8.91	1.1E-06	3.5E-07	1.1E-06				14%	-7.7	-8.2	-10.3
perylene-3,4:9,10-tetracarboxylic dianhydride	204-905-3	128-69-8	128698	1822	Reach_1112	1257	392	265.1	1.1E-11	3.1E-02	1.8E+06			3.5E-07	1.1E-08	3.5E-08				21%	-7.8	-8.2	-9.6
1-(1-methyl-2-propoxyethoxy)propan-2-ol	249-949-4	29911-27-1	29911271	2577	Reach_2636	1258	176	7.1	4.7E+00	4.8E+03	4.4E+00	15		3.5E-07	1.1E-07	3.5E-07				16%	-8.5	-8.2	-9.9
2,2'-iminobis[4,6-diamino-1,3,5-triazine]	222-695-1	3576-88-3	3576883	2746	Reach_1973	1259	235	210.4	5.2E-08	1.9E+04	2.4E+00		8.7	1.1E-07	1.1E-07	1.1E-07				19%	-7.3	-8.2	-9.8
{5-chloro-2-[(cyclopropylmethyl)amino]phenyl}(phenyl)methar	618-944-2	93413-69-5	93413695	1019	Reach_4503	1260	277	118.8	3.3E-05	7.1E+02	1.9E+03		6	3.9E-08	3.5E-07	1.1E-06				21%	-8.2	-8.2	-9.5
610-029-6	206-564-6	354-58-5	354585	2737	Reach_1248	1261	187	-75.2	4.5E+04	3.0E+02	1.2E+03			3.5E-08	1.1E-08	1.1E-08				14%	-7.1	-8.2	-10.3
2-(octylthio)ethanol	222-598-4	3547-33-9	3547339	613	Reach_1970	1262	190	39.1	4.2E-02	2.6E+01	2.4E+03	15		1.2E-07	3.5E-07	1.1E-06				19%	-8.5	-8.2	-9.7
N-[4-(aminocarbonyl)phenyl]-4-methoxy-3-nitrobenzamide	298-790-7	93839-20-4	93839204	4087	Reach_2999	1263	315	245.0	2.5E-10	3.4E+02	2.2E+01	14.1	14.5	1.1E-06	1.1E-07	3.5E-07				14%	-7.2	-8.2	-10.3
potassium O-isobutyl dithiocarbonate	676-405-7	165253-31-6	165253316	2097	Reach_4616	1264	101	-16.6	5.7E+02	1.6E+05	7.6E-01									18%	-7.9	-8.2	-9.9
2,6-dichlorobenzoxazole	210-557-3	618-62-2	618622	759	Reach_1438	1265	192	65.7	6.8E-01	8.0E+01	1.3E+03			4.6E-09	1.1E-08	3.5E-08				19%	-8.5	-8.2	-9.5
4-aminobenzoic acid	205-753-0	150-13-0	150130	2007	Reach_1203	1266	137	94.1	3.4E-03	2.0E+04	9.1E+00	5.01	11.6	1.1E-06	1.1E-07	3.5E-07				14%	-7.3	-8.2	-10.3
undecan-4-olide	203-225-4	104-67-6	104676	1398	Reach_626	1267	184	10.7	5.5E-01	5.8E+01	1.1E+03			3.5E-07	3.5E-08	1.1E-07				16%	-8.5	-8.2	-9.6
2-ethylhexyl cyanoacetate	236-425-5	13361-34-7	13361347	1870	Reach_2332	1268	197	43.6	3.4E-01	6.0E+01	7.8E+02			1.1E-06	3.5E-07	1.1E-06				15%	-8.5	-8.2	-9.9
butylamine	203-699-2	109-73-9	109739	263	Reach_787	1269	73	-58.8	1.3E+04	4.9E+05	6.8E+00		4	4.1E-07	3.5E-07	1.1E-06				16%	-8.5	-8.2	-9.5
S-allyl 5-amino-4-(2-methylphenyl)-3-oxo-2,3-dihydro-1H-pyra	203-472-8	107-20-0	107200	215	Reach_699	1270	78	-71.7	9.2E+03	5.7E+04	1.2E+00			8.1E-07	1.1E-07	3.5E-07				14%	-7.1	-8.2	-10.3
N-(1,1-dimethyl-3-oxobutyl)acrylamide	220-713-2	2873-97-4	2873974	2542	Reach_1879	1271	169	96.0	7.7E-02	1.1E+04	8.9E-01	14.6	14.8	1.1E-06	3.5E-07	1.1E-06				14%	-7.2	-8.2	-10.2
4,4'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[2,4-dihy	222-530-3	3520-72-7	3520727	2725	Reach_1969	1272	624	349.8	2.6E-21	1.4E-07	3.8E+10	5.72	12.6	3.5E-07	3.5E-08	3.5E-08				16%	-7.6	-8.2	-9.9
3,5-diacetamido-2,4,6-triiodobenzoic acid	202-815-9	100-06-1	100061	1291	Reach_549	1273	150	24.7	1.8E+00	3.3E+03	5.6E+01			1.1E-06	3.5E-07	1.1E-06				14%	-7.3	-8.2	-10.3
[2-[[2-cyano-3-[4-(diethylamino)phenyl]-1-oxoallyl]oxy]ethyl][3	278-859-8	78181-99-4	78181994	6036	Reach_2953	1274	636	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.9	-8.2	-9.9
1,3-diethyl-2-thiourea	203-308-5	105-55-5	105555	178	Reach_642	1275	132	24.3	9.2E+00	8.6E+04	4.0E+00	13	12	5.7E-09	3.5E-07	1.1E-06				23%	-7.8	-8.2	-9.2
cyclohexanediacetic acid	203-892-1	111-65-9	111659	306	Reach_863	1276	114	-68.5	2.0E+03	8.2E+00	1.9E+04			3.1E-07	3.5E-08	1.1E-07				14%	-7.6	-8.2	-10.2
2-({2-[(3-aminobenzoyl)amino]ethyl}sulfonyl)ethyl hydrogen su	220-040-4	2612-57-9	2612579	2455	Reach_1847	1277	188	24.2	1.5E+01	1.6E+02	7.6E+03			1.1E-07	1.1E-08	3.5E-08				14%	-7.0	-8.2	-10.3
(3S-cis)-3,6-dimethyl-1,4-dioxane-2,5-dione	213-243-4	931-87-3	931873	4064	Reach_1609	1278	110	-58.8	1.2E+03	2.4E+01	8.7E+03			3.5E-07	1.1E-07	3.5E-07				14%	-7.3	-8.2	-10.2
erythromycin thiocyanate	231-723-1	7704-67-8	7704678	1236	Reach_2271	1279	793	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.9	-8.2	-9.9
cyclopentane	206-016-6	287-92-3	287923	2545	Reach_1222	1280	70	-94.5	4.2E+04	3.5E+02	4.8E+02			3.5E-07	1.1E-07	3.5E-07				22%	-8.6	-8.2	-11.1
1-vinylhexahydro-2H-azepin-2-one	218-787-6	2235-00-9	2235009	2331	Reach_1777	1281	139	55.1	1.2E+00	1.1E+04	1.7E+01		14.4	1.1E-06	3.5E-07	1.1E-06				14%	-8.4	-8.2	-10.2
2,5-bis(p-toluidino)terephthalic acid	233-651-6	10291-28-8	10291288	1355	Reach_2287	1282	376	252.9	7.4E-11	9.4E-01	3.7E+05	3.7	14.5	1.1E-06	1.1E-07	3.5E-07				14%	-7.7	-8.2	-10.2
crotonaldehyde	224-030-0	4170-30-3	4170303	634	Reach_2018	1283	70	-80.6	4.2E+03	1.5E+05	4.0E+00			4.2E-06	1.1E-06	3.5E-06				14%	-8.5	-8.2	-9.8
2-chlorotoluene	202-424-3	95-49-8	95498	1030	Reach_430	1284	127	-27.5	3.5E+02	5.6E+01	1.5E+03			3.5E-09	3.5E-08	1.1E-07				24%	-8.6	-8.2	-10.6
ethyl cyanoacetate	203-309-0	105-56-6	105566	1415	Reach_643	1285	113	-10.9	2.9E+01	2.3E+04	1.0E+00			3.5E-06	3.5E-07	1.1E-06				14%	-8.5	-8.3	-10.2
4-[(5-{[(benzyloxy)carbonyl]amino}pentyl)(hydroxy)amino]-4-o	600-744-1	106410-46-2	106410462	1435	Reach_4073	1286	352	231.5	8.5E-12	2.6E+03	3.0E+01	4.67		1.1E-06	1.1E-07	3.5E-07				14%	-7.3	-8.3	-10.3
methyl hydrogen 2-nitroterephthalate	252-360-5	35092-89-8	35092898	2722	Reach_2686	1287	225	147.0	2.7E-04	6.6E+02	3.4E+01	2.95		1.1E-06	1.1E-07	3.5E-07				14%	-7.4	-8.3	-10.3
2,5-dimethoxyaniline	256-380-5	49564-57-0	49564570	2984	Reach_2762	1288	230	144.5	2.1E-04	1.2E+04	3.5E+00		12.3	1.1E-06	3.5E-07	1.1E-06				14%	-7.4	-8.3	-10.3
1,2,4-trimethylbenzene	202-436-9	95-63-6	95636	1035	Reach_436	1289	120	-22.5	2.2E+02	8.5E+01	4.3E+03			1.4E-08	3.5E-08	1.1E-07				23%	-8.5	-8.3	-10.3
7-methylenepentadecane	603-419-2	13043-55-5	13043555	1836	Reach_4119	1290	224	13.0	1.9E+00	1.4E-03	1.3E+08			1.1E-06	1.1E-07	3.5E-07				23%	-8.2	-8.3	-10.3
N,N,N',N'-tetramethyl-2,2'-oxybis(ethylamine)	221-220-5	3033-62-3	3033623	2592	Reach_1900	1291	160	-5.8	1.0E+02	2.6E+05	2.9E-01		4.98	1.1E-06	1.1E-07	3.5E-07				14%	-8.5	-8.3	-10.3
disodium 4,5-dichloro-2-[[4,5-dihydro-3-methyl-5-oxo-1-(3-sul	209-067-2	554-68-7	554687	5931	Reach_1363	1292	138	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.9	-8.3	-9.9
5-{5-chloro-3-[4-(methylsulfonyl)phenyl]pyridin-2-yl}-2-methyl	202-225-1	93-17-4	93174	4063	Reach_400	1293	177	75.2	1.3E-01	2.4E+03	1.6E+01									18%	-7.9	-8.3	-9.9
N-acetylsulphanilyl chloride	208-494-1	530-78-9	530789	3086	Reach_1327	1294	281	139.7	3.0E-04	3.6E+01	1.4E+05	4.19		1.1E-06	3.5E-07	1.1E-06				14%	-7.4	-8.3	-10.3
2-amino-2-methylpropanol	204-709-8	124-68-5	124685	1792	Reach_1081	1295	89	-8.5	6.6E+01	9.2E+05	1.8E-01	15	4.5	3.5E-06	1.1E-06	3.5E-06				14%	-8.3	-8.3	-10.2
tetrapropylammonium bromide	217-727-6	1941-30-6	1941306	5759	Reach_1736	1296	266	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-7.9	-8.3	-9.9
allyl (2S,4S)-4-(benzoylthio)-2-(dimethylcarbamoyl)pyrrolidine-	204-255-0	118-48-9	118489	1671	Reach_964	1297	163	76.7	1.0E-01	3.4E+03	4.0E+02			3.5E-06	3.5E-07	1.1E-06				14%	-7.4	-8.3	-10.3
9-ethylcarbazole	671-709-6	430-67-1	430671	2905	Reach_4615	1298	81	-94.9	9.7E+04	9.1E+05	4.6E-01			3.5E-06	1.1E-06	3.5E-06				16%	-8.5	-8.3	-10.1
6-(hydroxymethyl)-4-phenyl-3,4-dihydro-2H-chromen-2-ol	242-687-1	18936-17-9	18936179	2216	Reach_2472	1299	83	-57.6	1.7E+03	8.5E+03	1.8E+01			3.5E-07	1.1E-07	3.5E-07				14%	-7.2	-8.3	-10.3
benzenesulphonamide	202-637-1	98-10-2	98102	4178	Reach_498	1300	157	78.8	2.0E-02	5.1E+03	2.3E+00	10.1		3.5E-07	3.5E-08	1.1E-07				16%	-7.6	-8.3	-10.2
1,2-dibromoethane	203-444-5	106-93-4	106934	202	Reach_683	1301	188	-39.2	1.5E+03	3.7E+03	1.0E+02			1.4E-08	3.5E-08	1.1E-07				23%	-8.6	-8.3	-10.2
(2-hydroxyethyl)ammonium mercaptoacetate	204-815-4	126-97-6	126976	5647	Reach_1092	1302	153	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.3	-9.9
triethylammonium chloride	619-636-0	125971-57-5	125971575	1800	Reach_4534	1303	293	188.5	5.6E-07	1.1E+01	1.8E+04									18%	-8.0	-8.3	-9.9
2-(benzylmethylamino)ethyl acetoacetate	207-151-3	445-03-4	445034	2926	Reach_1276	1304	196	31.9	1.3E+01	1.1E+03	4.8E+02		10.1	1.1E-06	3.5E-07	1.1E-06				14%	-8.2	-8.3	-10.3
benzyl butyl phthalate	201-622-7	85-68-7	85687	968	Reach_299	1305	312	61.1	5.9E-03	2.3E+00	6.9E+04			7.5E-07	1.1E-07	3.5E-07				17%	-8.5	-8.3	-9.9
dibutyl phthalate	201-557-4	84-74-2	84742	963	Reach_290	1306	278	6.0	3.0E-02	1.5E+01	4.1E+04			8.9E-07	1.1E-07	3.5E-07				17%	-8.5	-8.3	-10.0
sodium 2-butyloctyl sulphate	303-553-9	94200-74-5	94200745	6090	Reach_3008	1307	288	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.3	-9.9
601-145-8	230-961-3	7384-80-7	7384807	3628	Reach_2245	1308	150	17.0	4.3E-01	1.3E+03	3.0E+02	15.7		1.1E-06	1.1E-07	3.5E-07				19%	-7.9	-8.3	-9.8
1,4-dimethoxybenzene	205-771-9	150-78-7	150787	484	Reach_1205	1309	138	-5.6	1.1E+01	2.7E+03	1.4E+02			7.3E-07	3.5E-07	1.1E-06				15%	-8.5	-8.3	-9.9
(1S)-1,2,3,4-tetrahydronaphthalen-1-amine	201-258-9	80-20-6	80206	3789	Reach_260	1310	264	190.2	1.8E-07	5.6E+02	1.7E+01		11	1.1E-06	3.5E-07	1.1E-06				16%	-8.5	-8.3	-9.8
(1R)-1,2,3,4-tetrahydronaphthalen-1-amine	617-178-6	80841-78-7	80841787	3799	Reach_4447	1311	149	60.2	8.8E-03	2.1E+03	6.2E+00			3.5E-07	3.5E-08	1.1E-07				16%	-8.5	-8.3	-9.8
D-glucono-1,5-lactone	202-016-5	90-80-2	90802	4006	Reach_367	1312	178	136.5	3.7E-07	1.5E+05	1.0E-02	11.4		3.5E-06	3.5E-07	1.1E-06				14%	-7.1	-8.3	-10.5
propylphosphonic acid	225-121-8	4672-38-2	4672382	2957	Reach_2054	1313	124	28.3	1.1E-02	1.5E+05	9.5E-01	2.6		1.1E-06	3.5E-07	1.1E-06				14%	-7.3	-8.3	-10.2
dimethyl sebacate	203-431-4	106-79-6	106796	1446	Reach_678	1314	230	-27.2	1.5E+00	9.7E+01	2.2E+03			3.5E-07	3.5E-08	1.1E-07				17%	-8.5	-8.3	-9.6
1,3-dichlorobenzene	208-792-1	541-73-1	541731	685	Reach_1341	1315	147	-14.3	1.8E+02	1.2E+02	1.9E+03			2.3E-09	1.1E-08	3.5E-08				24%	-8.6	-8.3	-10.3
methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	228-985-4	6386-38-5	6386385	3420	Reach_2176	1316	292	131.4	1.8E-04	2.8E+00	1.1E+05	11.9		3.5E-07	1.1E-07	3.5E-07				19%	-8.3	-8.3	-9.8
2,6-dichloro-N-phenylaniline	203-787-0	110-64-5	110645	1527	Reach_823	1317	88	-8.8	7.3E-01	2.5E+05	3.7E-01			3.5E-06	1.1E-06	3.5E-06				17%	-8.5	-8.3	-10.0
diethyl ether--boron trifluoride	201-265-7	80-26-2	80262	934	Reach_261	1318	196	21.5	6.6E+00	4.4E+02	2.2E+04			6.8E-07	3.5E-07	1.1E-06				18%	-8.0	-8.3	-9.9
succinic anhydride	203-570-0	108-30-5	108305	1481	Reach_739	1319	100	-52.8	2.4E-01	7.3E+03	6.5E+00			3.5E-06	3.5E-07	1.1E-06				14%	-8.1	-8.3	-10.3
sodium 3-mercaptopropanesulphonate	241-620-3	17636-10-1	17636101	5741	Reach_2438	1320	178	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.3	-9.9
619-799-8	614-977-1	69477-29-8	69477298	6002	Reach_4404	1321	1194	0.0												16%	-8.5	-8.3	-9.8
calcium bis[4-[[1-[[(2-chlorophenyl)amino]carbonyl]-2-oxoprop	276-057-2	71832-85-4	71832854	6011	Reach_2932	1322	920	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.3	-9.9
methyl myristate	210-412-4	615-16-7	615167	3336	Reach_1425	1323	134	95.8	4.9E-02	6.5E+02	1.6E+01			3.5E-07	3.5E-08	3.5E-07				21%	-8.5	-8.3	-10.2
difluoromethane	200-839-4	75-10-5	75105	3657	Reach_130	1324	52	-159.6	1.0E+06	9.1E+03	5.1E+00			3.5E-08	1.1E-08	1.1E-08				23%	-8.9	-8.3	-10.8
6,10-dimethylundeca-3,5,9-trien-2-one	205-457-1	141-10-6	141106	1932	Reach_1157	1325	192	5.8	2.6E+00	1.8E+01	2.7E+04			1.1E-06	3.5E-07	1.1E-06				17%	-8.5	-8.3	-9.9
pentane-1,5-diol	203-854-4	111-29-5	111295	1545	Reach_851	1326	104	3.3	5.6E-01	5.9E+05	1.9E+00	15.6		3.5E-06	1.1E-06	3.5E-06				14%	-7.5	-8.3	-10.2
601-329-8	247-832-2	26591-72-0	26591720	5806	Reach_2590	1327	222	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				19%	-7.6	-8.3	-9.9

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
2-phenylethanol	200-456-2	60-12-8	60128	3306	Reach_55	1328	122	5.8	3.2E+00	5.3E+03	3.7E+01	15.5		1.1E-06	3.5E-07	1.1E-06				14%	-8.5	-8.3	-10.1
2-chlorophenyl isocyanate	612-101-2	61203-94-9	61203949	3329	Reach_4371	1329	202	24.4	6.2E-01	4.4E-02	1.6E+06			3.5E-07	3.5E-08	1.1E-07				16%	-8.5	-8.3	-9.8
α-[2-(methylamino)ethyl]benzyl alcohol	207-223-4	454-31-9	454319	2940	Reach_1278	1330	124	-92.0	5.0E+03	2.3E+04	4.7E+00			3.5E-06	3.5E-07	1.1E-06				14%	-7.7	-8.3	-10.3
methyl (3R,5S,6E)-7-{4-(4-fluorophenyl)-6-isopropyl-2-[methyl(	201-757-1	87-61-6	87616	979	Reach_313	1331	181	16.4	9.6E+00	2.7E+01	8.5E+03			2.9E-09	1.1E-08	3.5E-08				14%	-7.6	-8.3	-10.3
2,6-difluoro-3-[(propylsulfonyl)amino]benzoic acid	700-740-0	1103234-56-5	1103234565	1517	Reach_4982	1332	279	167.0	3.4E-05	4.4E+02	2.2E+01	1.79		1.1E-06	1.1E-07	3.5E-07				14%	-7.4	-8.3	-10.3
2,4-dichloro-5-sulphamoylbenzoic acid	600-906-1	109232-37-3	109232373	1497	Reach_4076	1333	221	16.0	3.8E+00	1.5E+01	2.3E+04			3.5E-06	3.5E-07	1.1E-06				14%	-7.4	-8.3	-10.3
methyl 5-nitrohydrogen.isophthalate	217-793-6	1955-46-0	1955460	2235	Reach_1739	1334	225	147.0	2.7E-04	7.1E+02	3.4E+01	3.03		1.1E-06	1.1E-07	3.5E-07				14%	-7.4	-8.3	-10.3
3-amino-4-chlorobenzoic acid	695-654-2	1012341-48-8	1012341488	1316	Reach_4692	1335	381	218.6	1.5E-08	5.0E-01	6.0E+05	4.55		3.5E-07	3.5E-08	1.1E-07				14%	-7.4	-8.3	-10.3
2-chloro-N-(2,6-dichlorophenyl)-N-phenylacetamide	223-460-6	3905-19-9	3905199	2832	Reach_2000	1336	794	349.8	6.3E-32	1.2E-12	1.9E+13			3.5E-08	3.5E-09	1.1E-08				19%	-8.4	-8.3	-9.8
1,1,1,3,3,3-hexamethyldisilazane	213-668-5	999-97-3	999973	1096	Reach_1631	1337	161	-58.1	1.7E+03	3.0E+01	4.2E+02		3	8.4E-09	3.5E-09	3.5E-09				24%	-8.9	-8.3	-11.0
5-Chloro-1,3-dimethyl-1H-pyrazole-4-carbonyl chloride	203-907-1	111-78-4	111784	311	Reach_871	1338	108	-57.6	6.6E+02	8.4E+01	5.4E+03			1.5E-08	1.1E-07	3.5E-07				14%	-7.4	-8.3	-10.3
hexyl salicylate	228-408-6	6259-76-3	6259763	3375	Reach_2159	1339	222	99.7	3.3E-03	2.5E+01	1.1E+05	9.8		1.1E-06	1.1E-07	3.5E-07				18%	-8.4	-8.3	-10.0
octadecyl acrylate	225-383-3	4813-57-4	4813574	2971	Reach_2064	1340	325	98.5	1.1E-03	2.0E-04	1.2E+09			1.1E-06	1.1E-07	3.5E-07				23%	-8.2	-8.3	-9.7
2-amino-4-chlorophenol	604-434-7	144689-93-0	144689930	1978	Reach_4152	1341	240	154.4	4.0E-07	8.3E+02	7.4E+01	11.8	11.1	3.5E-06	3.5E-07	1.1E-06				14%	-7.4	-8.3	-10.3
619-779-9	607-657-8	252317-48-9	252317489	5796	Reach_4246	1342	489	0.0												14%	-7.4	-8.3	-10.3
methyl palmitate	203-966-3	112-39-0	112390	1586	Reach_903	1343	270	63.2	6.3E-02	7.4E-02	1.8E+07			1.1E-06	1.1E-07	3.5E-07				22%	-8.4	-8.3	-10.3
icos-1-ene	249-220-0	28783-41-7	28783417	5818	Reach_2624	1344	176	0.0												23%	-8.3	-8.3	-9.5
4-aminoazobenzene	600-261-6	101990-44-7	101990447	1333	Reach_4058	1345	186	87.7	1.1E-01	4.3E+05	4.6E-01		4.46	3.5E-07	3.5E-08	1.1E-07				22%	-8.1	-8.3	-9.4
4-amino-5-hydroxynaphthalene-2,7-disulphonic acid	800-428-5	1256387-74-2	1256387742	1798	Reach_5045	1346	392	222.8	7.8E-09	5.3E-02	5.5E+04	12.3	7.28	1.1E-06	1.1E-07	3.5E-07				14%	-7.0	-8.3	-10.3
2-amino-5-chlorophenol	604-568-6	147118-40-9	147118409	1995	Reach_4157	1347	496	271.2	1.4E-15	1.1E+00	5.8E+02	14.2	12.5	1.1E-06	1.1E-07	3.5E-07				14%	-7.4	-8.3	-10.3
608-385-2	600-141-3	1009-22-9	1009229	1311	Reach_4056	1348	232	118.9	5.1E-03	3.6E+02	4.3E+01	12.1		3.5E-07	1.1E-07	3.5E-07				14%	-7.3	-8.3	-10.3
(Z)-4-hydroxy-4-(6-methoxynaphthalen-2-yl)but-3-en-2-one	604-848-8	152402-98-7	152402987	2023	Reach_4164	1349	300	229.1	2.9E-09	1.7E+01	1.8E+03	12.1		1.1E-06	3.5E-08	1.1E-07				15%	-7.3	-8.3	-10.3
methyl carbamate	619-293-7	97845-60-8	97845608	4173	Reach_4512	1350	356	212.3	3.9E-08	3.8E+01	1.9E+01			3.5E-06	3.5E-07	1.1E-06				14%	-8.4	-8.3	-10.3
climbazole	253-775-4	38083-17-9	38083179	620	Reach_2715	1351	293	153.1	2.8E-05	5.7E+01	5.8E+03		7	1.2E-08	1.1E-07	3.5E-07				23%	-8.0	-8.3	-9.3
tetrapropylammonium hydroxide	224-800-6	4499-86-9	4499869	5889	Reach_2042	1352	203	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.3	-9.9
2-bromopropionic acid	202-063-1	91-35-0	91350	4015	Reach_375	1353	308	228.7	3.5E-10	1.2E+03	5.9E+00	4.21		3.5E-06	3.5E-07	1.1E-06				14%	-7.2	-8.3	-10.3
4-hydroxy-2,2,6,6-tetramethylpiperidine-1-ethanol	258-132-1	52722-86-8	52722868	3072	Reach_2787	1354	201	95.5	1.1E-03	8.6E+04	3.9E+00	14.7	5.52	3.5E-06	3.5E-07	3.5E-06				14%	-7.5	-8.3	-10.2
N,N-bis(2-hydroxyethyl)dodecanamide	204-393-1	120-40-1	120401	13	Reach_993	1355	287	161.6	9.0E-07	2.2E+01	7.8E+02	14.5	15	4.0E-07	3.5E-07	1.1E-06				16%	-7.7	-8.3	-10.1
Ethyl 2-amino-4,5-bis(2-methoxyethoxy)benzoate	700-551-3	179688-27-8	179688278	2161	Reach_4931	1356	313	152.4	3.6E-05	4.5E+02	7.1E+01		11.9	1.1E-06	1.1E-07	3.5E-07				14%	-7.5	-8.3	-10.3
lithium dodecyl sulphate	218-058-2	2044-56-6	2044566	5768	Reach_1749	1357	272	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.3	-10.0
propyl acetate	203-686-1	109-60-4	109604	258	Reach_779	1358	102	-69.3	4.7E+03	1.7E+04	2.3E+01			9.1E-07	3.5E-07	1.1E-06				15%	-8.6	-8.3	-10.0
dodecyl methacrylate	205-570-6	142-90-5	142905	465	Reach_1184	1359	254	33.9	1.9E-01	1.1E-01	4.8E+06			8.4E-07	1.1E-07	3.5E-07				22%	-8.5	-8.3	-10.5
bis(2,4-dichloro-5-nitrophenyl) carbonate	254-471-4	39489-75-3	39489753	2841	Reach_2725	1360	442	219.9	1.2E-08	3.4E-02	2.6E+05			3.5E-07	1.1E-08	3.5E-08				20%	-7.8	-8.3	-9.9
diethyl oxalate	202-464-1	95-92-1	95921	1042	Reach_447	1361	146	-95.3	9.7E+01	1.8E+04	2.5E+00			1.1E-06	3.5E-07	1.1E-06				14%	-8.5	-8.3	-9.9
isopropyl acetate	203-561-1	108-21-4	108214	233	Reach_734	1362	102	-81.1	8.1E+03	1.8E+04	1.9E+01			5.2E-07	3.5E-07	1.1E-06				16%	-8.6	-8.3	-10.1
2,2'-dithiodi(benzoic acid)	246-563-8	25013-16-5	25013165	1208	Reach_2558	1363	360	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				22%	-8.0	-8.3	-9.5
2,3-epoxypropyl neodecanoate	247-979-2	26761-45-5	26761455	2487	Reach_2593	1364	228	48.8	6.8E-01	9.4E+00	5.4E+03			3.5E-06	3.5E-07	1.1E-06				15%	-8.6	-8.3	-10.0
4-Nitrophenyl 1,3-thiazol-5-ylmethyl carbonate	204-503-8	121-88-0	121880	1737	Reach_1021	1365	154	109.7	3.6E-04	6.2E+03	9.8E+00		12.7	3.5E-06	1.1E-07	3.5E-07				14%	-7.6	-8.3	-10.3
ferrate(4-), hexakis(cyano-C)-, Et 2-[6-(ethylamino)-3-(ethylimir	223-772-2	4065-45-6	4065456	52	Reach_2009	1366	308	211.5	1.8E-09	3.2E+02	2.3E+00									18%	-8.0	-8.3	-10.0
benz[cd]indol-2(1H)-one	228-168-2	6153-05-5	6153055	1279	Reach_2154	1367	96	-21.5	6.7E+01	4.5E+04	7.8E+00	15.5		3.5E-06	1.1E-06	3.5E-06				14%	-7.6	-8.3	-10.3
611-813-0	229-653-1	6640-22-8	6640228	5979	Reach_2199	1368	432	0.0												14%	-8.5	-8.3	-10.3
619-518-9	700-349-5	33719-11-8	33719118	5849	Reach_4871	1369	445	0.0												14%	-7.6	-8.3	-10.3
[4-[p,p'-bis(dimethylamino)benzhydrylidene]cyclohexa-2,5-dier	265-449-9	65113-55-5	65113555	5970	Reach_2868	1370	725	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.3	-10.0
2,2-bis(hydroxymethyl)propionic acid	225-306-3	4767-03-7	4767037	1272	Reach_2063	1371	134	86.2	1.7E-04	8.8E+05	8.5E-02	4.02		3.5E-06	3.5E-07	1.1E-06				14%	-7.0	-8.3	-10.3
605-866-9	609-962-1	41851-59-6	41851596	2884	Reach_4317	1372	151	34.4	7.6E+00	6.1E+03	3.7E+01			1.1E-06	1.1E-07	3.5E-07				14%	-7.4	-8.3	-10.3
disodium 4,4'-bis[[4-anilino-6-[(2-hydroxyethyl)amino]-1,3,5-tr	267-400-7	67859-51-2	67859512	5989	Reach_2892	1373	390	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.3	-10.0
chloroethane	200-830-5	75-00-3	75003	3654	Reach_122	1374	65	-111.3	1.6E+05	1.2E+04	3.8E+01			1.1E-07	1.1E-08	3.5E-08				23%	-8.8	-8.3	-10.8
1,4-dioxacycloheptadecane-5,17-dione	203-347-8	105-95-3	105953	1422	Reach_652	1375	270	71.1	5.8E-05	1.8E+01	5.1E+04			1.1E-06	1.1E-07	3.5E-07				17%	-7.9	-8.3	-10.1
oxybenzone	205-031-5	131-57-7	131577	22	Reach_1122	1376	228	129.8	8.8E-04	1.4E+02	3.3E+03	9.73		3.8E-08	1.1E-07	3.5E-07				21%	-8.3	-8.3	-9.6
[[(phosphonomethyl)imino]bis[hexamethylenenitrilobis(methy	252-156-6	34690-00-1	34690001	2714	Reach_2680	1377	685	90.3	2.7E-09	2.9E+05	1.6E-06	-0.35	1.64	3.5E-07	3.5E-08	1.1E-07				16%	-7.2	-8.3	-10.3
diammonium [[N,N'-ethylenebis[N-(carboxylatomethyl)glycinat	241-883-4	17958-73-5	17958735	5745	Reach_2449	1378	873	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.3	-10.0
2,6-difluorobenzamide	202-150-4	92-36-4	92364	4032	Reach_384	1379	240	172.2	2.7E-06	8.9E+01	3.6E+03			1.1E-06	1.1E-07	3.5E-07				14%	-8.2	-8.3	-10.3
2,6-dichloro-4,8-dipiperidinopyrimido[5,4-d]pyrimidine	613-175-9	6318-09-8	6318098	1282	Reach_4383	1380	234	116.2	1.7E-03	7.8E+00	9.5E+03		8.9	3.5E-07	3.5E-08	1.1E-07				20%	-7.8	-8.3	-9.8
barbituric acid	200-658-0	67-52-7	67527	3495	Reach_83	1381	128	199.0	7.5E-08	1.4E+04	5.6E-02	4		3.5E-06	3.5E-07	1.1E-06				14%	-7.0	-8.3	-10.4
peracetic acid	201-186-8	79-21-0	79210	917	Reach_235	1382	76	-42.3	3.2E+03	3.8E+05	8.5E-02	8.2		4.5E-06	3.5E-07	1.1E-06				14%	-8.5	-8.3	-10.1
(2S)-[(tert-butoxycarbonyl)amino](3-hydroxytricyclo[3.3.1.13,7	700-361-0	361442-00-4	361442004	2760	Reach_4874	1383	325	177.7	1.1E-07	6.5E-01	3.5E+02	3.44		1.1E-06	1.1E-07	3.5E-07				14%	-7.7	-8.3	-10.3
3-ethoxy-4-hydroxybenzaldehyde	204-464-7	121-32-4	121324	368	Reach_1010	1384	166	81.4	3.9E-02	5.9E+03	3.5E+01	7.3		6.6E-07	3.5E-07	1.1E-06				15%	-8.0	-8.3	-10.2
diisopropyl ether	203-560-6	108-20-3	108203	232	Reach_733	1385	102	-99.0	2.0E+04	8.8E+03	7.6E+01			2.2E-09	1.1E-07	3.5E-07				24%	-8.6	-8.3	-10.5
icosyl acrylate	200-424-8	59-42-7	59427	3275	Reach_50	1386	167	87.7	3.0E-03	1.7E+04	6.2E-01			1.1E-05	1.1E-06	3.5E-06				23%	-8.4	-8.3	-9.4
N,N-dimethyl-p-toluidine	202-805-4	99-97-8	99978	1094	Reach_544	1387	135	-6.6	2.8E+01	1.7E+03	5.2E+02		9	1.2E-08	1.1E-07	3.5E-07				23%	-8.6	-8.3	-9.4
isophthaloyl dichloride	202-774-7	99-63-8	99638	4214	Reach_535	1388	203	68.2	6.3E-01	6.9E+02	7.6E+00			3.5E-06	3.5E-07	1.1E-06				14%	-8.6	-8.3	-10.2
tributylmethylammonium chloride	260-135-8	56375-79-2	56375792	5935	Reach_2815	1389	236	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.3	-10.0
disodium 4-amino-3,6-bis[[4-[(2,4-diaminophenyl)azo]phenyl]a	229-208-1	6428-31-5	6428315	5967	Reach_2185	1390	840	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.3	-10.0
4'-chloro-2',5'-dimethoxyacetoacetanilide	224-638-6	4433-79-8	4433798	2922	Reach_2035	1391	272	174.2	1.2E-05	7.2E+02	1.8E+01	10.7	14.7	1.1E-06	1.1E-07	1.1E-06				14%	-7.4	-8.3	-10.3
[nitrilotris(methylene)]trisphosphonic acid, ammonium salt	603-981-9	136890-12-5	136890125	1903	Reach_4135	1392	355	165.7	1.0E-08	3.8E-02	7.1E+06									18%	-8.0	-8.3	-10.0
1-hydroxy-4-methyl-6-(2,4,4-trimethylpentyl)pyridin-2(1H)-one	202-874-0	100-64-1	100641	135	Reach_566	1393	113	-9.2	1.5E+00	4.4E+04	8.1E+00									18%	-8.0	-8.3	-10.0
sodium 2-amino-4,6-dinitrophenoxide	203-960-0	112-33-4	112334	1583	Reach_898	1394	163	56.8	6.7E-02	9.9E+06	2.1E-02									18%	-8.0	-8.3	-10.0
hexamethylene diacrylate	235-921-9	13048-33-4	13048334	1837	Reach_2320	1395	226	-29.7	2.2E+00	2.1E+02	1.2E+03			1.1E-06	1.1E-07	3.5E-07				15%	-8.6	-8.3	-9.9
potassium O-ethyl dithiocarbonate	203-552-2	108-12-3	108123	1476	Reach_730	1396	121	-54.0	3.2E+03	3.7E+03	8.5E+00									18%	-8.0	-8.3	-10.0
N-(2-ethylhexyl)-1-[[2-methyl-4-[(2-methylphenyl)azo]phenyl]a	204-436-4	120-93-4	120934	367	Reach_1006	1397	86	35.6	1.7E+00	3.7E+04	1.8E-01		14	3.7E-07	3.5E-07	1.1E-06				24%	-8.5	-8.3	-8.8
(3R)-3-amino-1-[3-(trifluoromethyl)-5,6-dihydro[1,2,4]triazolo[	213-063-6	921-03-9	921039	4027	Reach_1591	1398	161	-13.3	1.9E+02	1.1E+03	2.8E+00		0	1.1E-07	1.1E-08	3.5E-08				19%	-7.7	-8.3	-9.9
608-591-2	608-591-2	31221-06-4	31221064	5838	Reach_4279	1399	308	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.3	-10.0
zinc distearate	209-151-9	557-05-1	557051	5933	Reach_1371	1400	632	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.3	-10.0
Methyl 3-cyclopentyl-1-methyl-1H-indole-6-carboxylate	700-133-0	2436-29-5	2436295	2389	Reach_4774	1401	203	177.3	7.3E-06	2.1E+03	1.0E+01			1.1E-06	1.1E-07	3.5E-07				17%	-8.4	-8.3	-10.1
sodium N-(2-carboxyethyl)-N-dodecyl-β-alaninate	203-650-5	109-13-7	109137	1494	Reach_771	1402	160	-31.4	3.7E+02	7.3E+02	2.2E+02									18%	-8.0	-8.3	-10.0

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
pent-1-ene	203-694-5	109-67-1	109671	1506	Reach_784	1403	70	-108.4	7.1E+04	5.0E+02	4.6E+02			1.1E-06	1.1E-07	3.5E-07				20%	-8.6	-8.3	-11.3
ampicillin	239-477-7	15458-48-7	15458487	2037	Reach_2388	1404	195	172.8	2.5E-07	6.0E+04	3.4E-01	14.9	14.7	3.5E-06	3.5E-07	1.1E-06				20%	-7.7	-8.3	-9.7
2-ethoxyethanol	203-804-1	110-80-5	110805	284	Reach_829	1405	90	-44.2	4.1E+02	7.3E+05	3.8E-01	15		1.0E-06	3.5E-07	1.1E-06				14%	-8.5	-8.3	-10.2
2-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)pheno	274-570-6	70321-86-7	70321867	3559	Reach_2916	1406	448	259.2	2.2E-12	1.3E-03	4.7E+07	10.3	15.2	3.5E-07	3.5E-08	1.1E-07				16%	-7.9	-8.3	-10.2
[1-(4-bromobenzyl)-2-butyl-4-chloro-1H-imidazol-5-yl]methanc	604-770-4	151012-31-6	151012316	2016	Reach_4162	1407	358	198.6	3.0E-09	2.1E+00	8.9E+04	15.4	10.5	1.1E-06	1.1E-07	3.5E-07				14%	-7.7	-8.3	-10.3
dilactide	202-468-3	95-96-5	95965	4140	Reach_448	1408	144	26.1	2.1E-02	1.5E+07	4.5E+01			3.5E-06	3.5E-07	1.1E-06				14%	-7.4	-8.3	-10.3
aminoguanidinium hydrogen carbonate	219-956-7	2582-30-1	2582301	5800	Reach_1842	1409	136	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.3	-10.0
N-[3-(isodecyloxy)propyl]propane-1,3-diamine	276-432-0	72162-46-0	72162460	3598	Reach_2934	1410	272	105.4	3.7E-03	6.9E-01	7.9E+03		3.68	3.5E-07	3.5E-08	1.1E-07				17%	-8.6	-8.3	-9.8
trizinc dicitrate	208-901-2	546-46-3	546463	5926	Reach_1355	1411	574	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.3	-10.0
3,5,5-trimethylhexanal	226-603-0	5435-64-3	5435643	3140	Reach_2112	1412	142	-35.5	1.8E+02	7.3E+01	1.2E+03			1.1E-06	3.5E-07	1.1E-06				18%	-8.6	-8.3	-10.7
pentane-1,2-diol	226-285-3	5343-92-0	5343920	3102	Reach_2100	1413	104	-9.5	7.1E-01	5.4E+04	1.6E+00	14.9		3.5E-06	1.1E-06	3.5E-06				14%	-8.0	-8.3	-10.3
4-amino-5-methoxy-N,2-dimethylbenzenesulphonamide	203-040-9	102-56-7	102567	1345	Reach_593	1414	153	54.3	3.6E-01	9.0E+03	1.7E+01		10.1	1.1E-06	1.1E-07	3.5E-07				14%	-7.4	-8.3	-10.3
1,1'-binaphthyl-8,8'-dicarboxylic acid	700-688-9	111360-16-8	111360168	297	Reach_4968	1415	92	-59.2	3.2E+03	4.6E+02	3.5E+02	0		9.3E-07	3.5E-08	1.1E-07				19%	-8.1	-8.3	-9.9
604-759-4	604-759-4	150928-21-5	150928215	2015	Reach_4161	1416	807	327.4	5.0E-16	3.9E-02	6.9E+01	10.8		1.1E-06	1.1E-07	3.5E-07				14%	-7.4	-8.3	-10.3
5-difluoromethoxy-2-[[(3,4-dimethoxy-2-pyridyl)methyl]thio]-1	700-086-6	3159-04-4	3159044	1258	Reach_4756	1417	262	182.0	3.7E-06	5.4E+00	2.5E+03	14.6	13.4	3.5E-07	3.5E-08	1.1E-07				14%	-7.6	-8.3	-10.3
4,4'-azo-3-hydroxynaphthalene-1-sulphonate	600-593-1	104632-26-0	104632260	1396	PharmaBeta_621	1418	211	127.4	2.1E-03	5.8E+03	2.2E+02			3.5E-06	1.1E-07	3.5E-07				14%	-7.2	-8.3	-10.3
2-Methoxy-6-methylbenzoic acid	612-182-4	6161-65-5	6161655	3342	Reach_4373	1419	166	83.6	7.7E-02	1.6E+03	2.5E+01	3.8		1.1E-06	3.5E-07	1.1E-06				14%	-7.6	-8.3	-10.3
4-acetylmorpholine	216-913-4	1696-20-4	1696204	2118	Reach_1709	1420	129	27.4	1.8E+01	2.3E+05	1.3E-01		15	1.1E-06	3.5E-07	1.1E-06				14%	-7.2	-8.3	-10.3
{[2-(trifluoromethyl)benzoyl]amino}methyl acetate	619-484-5	895525-72-1	895525721	3978	Reach_4523	1421	220	55.6	3.2E-01	2.1E+02	6.8E+03			1.1E-06	1.1E-07	3.5E-07				15%	-8.6	-8.3	-10.1
pleuromulin	204-747-5	125-65-5	125655	1799	Reach_1084	1422	379	200.9	1.6E-09	9.2E-01	8.5E+02	12.6		1.1E-06	1.1E-07	3.5E-07				15%	-7.5	-8.3	-10.2
5-nitroisophthalic acid	210-568-3	618-88-2	618882	3358	Reach_1440	1423	211	169.2	2.4E-05	3.7E+03	3.7E+01	2.73		3.5E-06	1.1E-07	3.5E-07				14%	-7.4	-8.3	-10.5
2-(2-butoxyethoxy)ethyl 6-propylpiperonyl ether	200-076-7	51-03-6	51036	667	Reach_12	1424	338	152.7	7.0E-04	3.1E+00	1.9E+04			5.6E-07	1.1E-07	3.5E-07				17%	-8.5	-8.3	-10.1
2,2'-oxybis[5,5-dimethyl-1,3,2-dioxaphosphorinane] 2,2'-disulp	223-829-1	4090-51-1	4090511	2866	Reach_2012	1425	346	-19.8	3.6E-03	5.5E+00	3.3E+04			3.5E-07	1.1E-07	3.5E-07				18%	-8.5	-8.3	-10.0
methyl 3-mercaptopropionate	220-912-4	2935-90-2	2935902	2563	Reach_1888	1426	120	-40.3	2.5E+02	5.0E+04	6.5E+00	9.6		3.5E-06	3.5E-07	1.1E-06				14%	-8.6	-8.3	-10.1
2-{[(4-chloro-3-methoxypyridin-2-yl)methyl]sulfanyl}-6-(difluor	218-370-9	2135-17-3	2135173	532	Reach_1760	1427	410	215.7	1.4E-11	3.3E+01	3.9E+01	13		1.1E-07	3.5E-07	1.1E-06				14%	-7.7	-8.3	-10.3
4-(6-methylbenzothiazol-2-yl)aniline	207-141-9	443-83-4	443834	2924	Reach_1275	1428	145	-22.4	4.4E+02	7.7E+01	2.5E+03			3.5E-07	3.5E-08	1.1E-07				14%	-7.8	-8.3	-10.3
ethane-1,2-diyl palmitate	210-826-5	624-03-3	624033	3368	Reach_1451	1429	539	165.1	2.0E-07	1.2E-08	1.4E+14			1.1E-06	1.1E-07	3.5E-07				24%	-8.6	-8.3	-8.1
sodium 1H-benzotriazolide	239-269-6	15217-42-2	15217422	5711	Reach_2379	1430	141	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.3	-10.0
2-ethylhexyl 4-methoxycinnamate	226-775-7	5466-77-3	5466773	3151	Reach_2117	1431	290	99.9	1.8E-03	1.8E-01	6.3E+05			1.1E-06	1.1E-07	3.5E-07				19%	-8.5	-8.3	-9.9
2,4,6-trimethylbenzoyl chloride	208-235-2	517-23-7	517237	3044	Reach_1321	1432	128	12.7	4.1E+00	3.5E+04	3.5E-02			3.5E-06	3.5E-07	1.1E-06				16%	-8.6	-8.3	-9.7
1-methylimidazole	200-540-9	62-54-4	62544	6274	PharmaBeta_363	1433	158	0.0	0.0E+00	0.0E+00	0.0E+00		0	0.0E+00	0.0E+00	0.0E+00				16%	-8.6	-8.3	-10.1
2,5-dimethylhexyne-2,5-diol	700-314-4	82966-34-5	82966345	3838	Reach_4856	1434	420	189.0	1.3E-06	3.2E+00	1.1E+03			1.1E-07	1.1E-08	3.5E-08				14%	-7.4	-8.3	-10.3
Methyl 4-(butylamino)benzoate	629-348-7	23357-52-0	23357520	2350	Reach_4591	1435	147	48.0	2.7E+00	7.5E+02	2.6E+02		4.7	3.5E-07	3.5E-08	1.1E-07				14%	-7.8	-8.3	-10.4
N-phenylmaleimide	203-604-4	108-67-8	108678	242	Reach_751	1436	120	-22.5	2.7E+02	8.5E+01	4.3E+03			6.3E-09	3.5E-08	1.1E-07				14%	-7.5	-8.3	-10.3
N1-methyl-4-(methylsulfonyl)benzene-1,2-diamine	615-907-2	73097-51-5	73097515	3613	Reach_4418	1437	200	131.8	1.1E-03	1.4E+04	1.9E-01		12.2	1.1E-06	1.1E-07	1.1E-06				14%	-7.2	-8.3	-10.3
4-(Methylamino)-3-nitrobenzoic acid	249-050-7	28479-22-3	28479223	2533	Reach_2618	1438	168	11.5	2.7E+01	2.5E+03	6.0E+03			1.1E-06	1.1E-07	3.5E-07				14%	-7.4	-8.3	-10.6
2-methylaminoethanol	203-710-0	109-83-1	109831	1510	Reach_793	1439	75	-35.8	1.1E+02	1.0E+06	7.1E-02	15	4.1	3.5E-06	1.1E-06	3.5E-06				14%	-8.4	-8.4	-10.3
EPTC (reach)	212-073-8	759-94-4	759944	869	Reach_1529	1440	189	60.5	5.0E-01	1.6E+02	1.0E+03		14	2.6E-07	3.5E-08	3.5E-07				17%	-8.6	-8.4	-9.9
639-566-4	639-566-4	165184-98-5	165184985	2096	Reach_4605	1441	216	44.4	7.1E-02	1.1E+00	6.6E+04			1.1E-06	1.1E-07	3.5E-07				17%	-8.6	-8.4	-9.8
2-(4-aminophenyl)-6-methylbenzothiazole-7-sulphonic acid	696-374-3	100930-72-1	100930721	1312	Reach_4716	1442	326	184.0	1.7E-08	1.8E-02	1.1E+08	7.6		3.5E-07	3.5E-08	1.1E-07				14%	-7.3	-8.4	-10.3
dimethyl malonate	203-597-8	108-59-8	108598	1486	Reach_749	1443	132	-107.6	1.2E+02	1.2E+05	8.1E-01	13		3.5E-06	3.5E-07	1.1E-06				14%	-8.6	-8.4	-10.3
dimethylcarbamoyl chloride	202-810-1	100-01-6	100016	120	Reach_547	1444	138	71.6	2.8E-03	1.2E+03	3.0E+01		13	2.2E-09	1.1E-07	3.5E-07				14%	-8.6	-8.4	-10.3
didecylamine	214-312-1	1120-49-6	1120496	1571	Reach_1659	1445	298	94.5	2.7E-03	2.1E-03	4.7E+08		3.1	1.1E-06	1.1E-07	3.5E-07				23%	-8.2	-8.4	-9.9
689-404-1	607-145-4	227197-72-0	227197720	2337	Reach_4233	1446	154	49.5	3.9E+00	6.3E+02	2.3E+02		14.1	1.1E-07	1.1E-08	3.5E-08				14%	-7.3	-8.4	-10.3
tert-butyl-4-methoxyphenol	204-352-8	119-80-2	119802	357	Reach_987	1447	306	213.6	4.0E-09	1.7E+01	2.4E+03									18%	-8.0	-8.4	-10.0
3,4-dihydro-2-methoxy-2H-pyran	202-797-2	99-88-7	99887	4221	Reach_541	1448	135	23.2	1.3E+01	2.5E+02	3.4E+02			1.1E-06	1.1E-07	3.5E-07				15%	-8.6	-8.4	-10.0
4-aminotoluene-3-sulphonic acid	201-831-3	88-44-8	88448	3956	Reach_323	1449	187	139.2	9.4E-06	8.4E+03	3.0E-02	-0.93	11.2	3.5E-06	1.1E-07	3.5E-07				14%	-7.1	-8.4	-10.6
1H-2-Benzopyran-1,4(3H)-dione	616-178-3	75028-24-9	75028249	3656	Reach_4425	1450	216	160.6	8.5E-05	1.1E+04	9.1E+01			3.5E-06	3.5E-07	1.1E-06				14%	-7.8	-8.4	-10.3
ethyl 2-[3-formyl-4-(2-methylpropoxy)phenyl]-4-methyl-1,3-thi	256-376-3	49562-28-9	49562289	649	Reach_2761	1451	361	157.7	8.3E-05	5.3E-02	1.5E+05			6.0E-08	1.1E-07	1.1E-06				14%	-7.9	-8.4	-10.3
3-methyl-1-vinyl-1H-imidazolium methyl sulphate	222-294-1	3407-42-9	3407429	2689	Reach_1956	1452	236	87.6	1.6E-03	2.1E+01	3.2E+05									18%	-8.1	-8.4	-10.0
N-isopropyl-N'-phenyl-p-phenylenediamine	202-969-7	101-72-4	101724	1326	Reach_581	1453	226	104.4	9.5E-03	1.3E+01	1.9E+03		9.4	3.5E-06	1.1E-07	3.5E-07				14%	-7.8	-8.4	-10.4
trisodium 6,6',6''-(1,3,5-triazine-2,4,6-triyltriimino)trihexanoate	700-292-6	135043-68-4	135043684	5672	Reach_4846	1454	535	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.0	-8.4	-10.0
octacos-1-ene	260-124-8	56358-09-9	56358099	3191	Reach_2813	1455	494	254.8	5.5E-11	2.9E-04	9.3E+11			1.1E-06	1.1E-07	3.5E-07				24%	-8.7	-8.4	-8.7
cyclohexanecarboxylic acid	202-711-3	98-89-5	98895	1078	Reach_523	1456	128	43.5	7.6E+00	5.5E+03	2.3E+02	4.9		9.3E-07	3.5E-07	1.1E-06				15%	-8.1	-8.4	-10.3
β-alanine	203-536-5	107-95-9	107959	1472	Reach_722	1457	89	256.3	3.2E-05	6.6E+05	8.1E-05	3.7	3.7	3.5E-06	3.5E-07	1.1E-06				14%	-7.1	-8.4	-10.5
methyl cyanoacetate	203-288-8	105-34-0	105340	1412	Reach_638	1458	99	-22.6	4.7E+01	1.2E+05	3.4E-01			3.5E-06	3.5E-07	1.1E-06				14%	-8.6	-8.4	-10.4
acetaldehyde oxime	203-479-6	107-29-9	107299	218	Reach_703	1459	59	-73.6	7.4E+02	7.4E+04	6.2E-01	11.9		4.2E-07	3.5E-08	3.5E-07				16%	-8.6	-8.4	-9.8
tris[4-(diethylamino)phenyl]methylium acetate	263-974-8	63157-72-2	63157722	5960	Reach_2856	1460	516	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.1	-8.4	-10.0
glycollic acid	201-180-5	79-14-1	79141	3766	Reach_232	1461	76	23.3	2.3E+00	3.9E+05	8.5E-02	3.8		3.5E-06	3.5E-07	1.1E-06				14%	-7.2	-8.4	-10.4
methyl chloroformate	201-187-3	79-22-1	79221	3768	Reach_236	1462	94	-82.1	1.7E+04	2.7E+04	1.4E+00			1.1E-06	3.5E-07	1.1E-06				15%	-8.7	-8.4	-10.3
theophylline	600-476-5	1037184-07-8	1037184078	1377	Reach_4065	1463	288	164.2	1.0E-05	4.0E+00	6.3E+03	12.9		3.5E-07	3.5E-08	1.1E-07				23%	-7.6	-8.4	-9.4
ethyl acetoacetate	205-516-1	141-97-9	141979	459	Reach_1170	1464	130	-19.2	1.2E+02	2.0E+04	6.3E-01	10.6		1.1E-06	3.5E-07	1.1E-06				14%	-8.6	-8.4	-10.0
methyl [(2S,3S)-4-chloro-3-hydroxy-1-phenylbutan-2-yl]carbam	700-854-0	256473-04-8	256473048	2441	Reach_5014	1465	212	22.5	5.0E+01	2.3E+02	2.8E+02			1.1E-06	1.1E-07	3.5E-07				14%	-7.5	-8.4	-10.4
ethyl (2R)-2-hydroxy-4-phenylbutanoate	210-195-6	609-66-5	609665	3321	Reach_1416	1466	156	102.1	7.9E-03	4.6E+02	4.5E+00	14.1		3.5E-07	3.5E-08	1.1E-07				14%	-7.7	-8.4	-10.3
ethyl 2-ethoxy-1-{[2'-(1H-tetrazol-5-yl)biphenyl-4-yl]methyl}-1H	200-825-8	74-96-4	74964	843	Reach_119	1467	109	-92.1	6.2E+04	6.7E+03	4.7E+01			9.7E-09	1.1E-07	3.5E-07				14%	-7.8	-8.4	-10.3
hexacos-1-ene	210-743-4	622-58-2	622582	3365	Reach_1446	1468	133	-19.2	1.3E+02	2.2E+03	1.4E+03			1.1E-06	3.5E-07	1.1E-06				24%	-8.7	-8.4	-9.1
3,3'-[(2-chloro-5-methyl-p-phenylene)bis[imino(1-acetyl-2-oxo	213-059-4	920-66-1	920661	1011	Reach_1590	1469	168	-95.6	2.1E+04	7.5E+03	1.3E+01	8.83	0	1.4E-07	3.5E-07	1.1E-06				22%	-8.0	-8.4	-9.6
2-methyl-2-propylpropane-1,3-diol	249-942-6	29901-62-0	29901620	5827	Reach_2635	1470	211	0.0												14%	-8.3	-8.4	-10.3
1,2-benzisothiazol-3(2H)-one 1,1-dioxide	210-852-7	624-54-4	624544	3370	Reach_1453	1471	144	-32.6	2.2E+02	9.4E+02	6.8E+02	0	0	3.5E-06	3.5E-07	1.1E-06				22%	-7.9	-8.4	-9.6
1,4-dimethoxy-2-nitrobenzene	201-903-4	89-39-4	89394	3973	Reach_342	1472	183	73.6	2.8E-01	1.4E+03	9.3E+01			1.1E-06	1.1E-07	3.5E-07				14%	-8.6	-8.4	-10.3
4-chloro-3,5-dinitro-α,α,α-trifluorotoluene	206-889-3	393-75-9	393759	2839	Reach_1265	1473	271	101.9	5.1E-02	6.0E-01	1.7E+03			1.1E-06	3.5E-08	1.1E-07				15%	-8.6	-8.4	-10.0
2-chloro-N,N-dimethyl-3-oxobutyramide	227-372-9	5810-11-7	5810117	1278	Reach_2137	1474	164	47.4	2.4E+00	2.5E+06	8.5E-01	6.19		3.5E-07	1.1E-07	3.5E-07				16%	-7.5	-8.4	-10.3
1,1'-dithiobis[hexahydro-2H-azepin-2-one]	250-056-7	30113-45-2	30113452	2586	Reach_2642	1475	215	51.3	4.6E-01	4.7E+02	8.3E+03		4.1	3.5E-07	3.5E-08	1.1E-07				16%	-7.4	-8.4	-10.3
1,4:3,6-dianhydro-D-glucitol	211-492-3	652-67-5	652675	3449	Reach_1488	1476	146	60.5	4.1E-02	4.9E+04	1.2E-01	13.7		1.1E-06	3.5E-07	1.1E-06				14%	-7.5	-8.4	-10.4
1,1-difluoroethylene	200-867-7	75-38-7	75387	3670	Reach_143	1477	64	-156.3	2.5E+06	2.2E+03	1.7E+01			1.1E-06	1.1E-07	3.5E-07				20%	-8.8	-8.4	-11.3

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
606-738-5	200-709-7	69-53-4	69534	808	Reach_94	1478	349	324.9	3.8E-11	3.5E+03	2.8E+01		7	5.5E-08	1.1E-07	3.5E-07				19%	-7.7	-8.4	-10.0
3-amino-4-hydroxy-N-phenylbenzenesulphonamide	202-847-3	100-39-0	100390	1304	Reach_554	1479	171	-8.9	4.6E+01	2.0E+02	7.6E+02			3.5E-07	3.5E-08	1.1E-07				14%	-7.5	-8.4	-10.3
diammonium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](	217-440-6	1852-04-6	1852046	2195	Reach_1726	1480	216	135.0	4.2E-04	1.1E+03	4.8E+02									18%	-8.1	-8.4	-10.0
4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)phen	233-215-5	10081-67-1	10081671	1310	Reach_2280	1481	406	214.5	2.3E-08	2.1E-04	3.2E+08		13.2	1.1E-06	3.5E-07	1.1E-06				15%	-7.5	-8.4	-10.2
5-ethyl-2-methylpyridine	203-250-0	104-90-5	104905	172	Reach_632	1482	121	4.3	1.4E+02	8.3E+04	2.5E+02		8	1.1E-08	3.5E-08	1.1E-07				23%	-8.6	-8.4	-9.4
607-936-4	224-339-0	4316-74-9	4316749	5886	Reach_2028	1483	161	0.0												14%	-7.5	-8.4	-10.4
8-isopropyl-8-azabicyclo[3.2.1]octan-3-one	620-037-1	99636-38-1	99636381	4213	Reach_4557	1484	89	-52.1	5.4E+03	2.0E+05	3.2E-01		4.5	1.1E-06	1.1E-07	3.5E-07				14%	-8.6	-8.4	-10.3
methyl 2-naphthyl ether	202-213-6	93-04-9	93049	1017	Reach_397	1485	158	38.4	3.6E-01	7.9E+01	1.8E+03			1.1E-08	1.1E-07	3.5E-07				23%	-8.7	-8.4	-9.5
disodium (Z)-4-(9-octadecenylamino)-4-oxo-2(or 3)-sulphonatc	261-222-3	58353-68-7	58353687	5940	Reach_2828	1486	492	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.1	-8.4	-10.0
5,12-dihydroquino[2,3-b]acridine-7,14-dione	213-879-2	1047-16-1	1047161	1400	Reach_1636	1487	312	218.5	1.5E-08	2.4E-02	2.4E+01	14.5	8.15	1.1E-06	3.5E-07	1.1E-06				14%	-7.6	-8.4	-10.3
611-622-2	616-212-7	75330-75-5	75330755	856	Reach_4428	1488	405	197.8	1.8E-10	5.2E-01	5.5E+04	14.6		2.5E-07	1.1E-07	3.5E-07				15%	-7.5	-8.4	-10.3
2-[(4-chloro-2-nitrophenyl)azo]-N-(2,3-dihydro-2-oxo-1H-benzi	235-462-4	12236-62-3	12236623	1747	Reach_2307	1489	417	284.3	5.2E-13	1.3E+01	1.8E+03	8.58	12.1	1.1E-06	3.5E-08	1.1E-07				14%	-7.7	-8.4	-10.5
trimethyloctadecylammonium chloride	203-929-1	112-03-8	112038	5610	Reach_885	1490	348	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.1	-8.4	-10.0
619-682-1	211-932-4	713-95-1	713951	3581	Reach_1521	1491	198	18.7	1.3E-01	3.8E+01	3.5E+03	0	0	3.5E-07	3.5E-08	1.1E-07				19%	-7.6	-8.4	-10.0
2-hexyloxyethanol	203-951-1	112-25-4	112254	1580	Reach_893	1492	146	2.6	6.1E+00	8.5E+03	3.5E+01	15		3.5E-06	1.1E-06	3.5E-06				14%	-8.6	-8.4	-10.3
618-965-7	616-640-4	78628-80-5	78628805	6038	Reach_4442	1493	328	0.0												14%	-7.5	-8.4	-10.4
O-(4-bromo-2-chlorophenyl) O-ethyl S-propyl phosphorothioat	217-983-9	2031-67-6	2031676	2259	Reach_1746	1494	178	-23.2	7.7E+02	1.7E+03	6.3E+00			1.1E-06	3.5E-07	1.1E-06				23%	-8.6	-8.4	-9.5
(carboxymethyl)dimethyl-3-[(1-oxododecyl)amino]propylamm	224-292-6	4292-10-8	4292108	1267	Reach_2026	1495	343	283.0	6.4E-13	1.7E-02	4.9E+02	1.87	15.5	1.1E-06	1.1E-07	3.5E-07				14%	-7.7	-8.4	-10.4
lithium 2-methoxy-4-(trifluoromethyl)pyridine-3-thiolate	617-976-4	871544-06-8	871544068	6072	Reach_4483	1496	210	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.1	-8.4	-10.0
606-819-5	606-819-5	216699-04-6	216699046	5773	Reach_4219	1497	418	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.1	-8.4	-10.0
2,2'-[ethylenebis(oxyphenyl-2,1-eneazo)]bis[N-(2,3-dihydro-2-c	278-770-4	77804-81-0	77804810	3736	Reach_2951	1498	733	349.8	2.6E-26	3.5E-03	1.7E+04	8.42	11.6	3.5E-07	3.5E-08	1.1E-07				16%	-8.8	-8.4	-10.3
benzonitrile	202-855-7	100-47-0	100470	128	Reach_560	1499	103	-7.5	7.5E+01	4.2E+03	3.5E+01			4.0E-07	3.5E-08	1.1E-07				16%	-8.6	-8.4	-9.7
4-nitro-o-anisidine	202-588-6	97-52-9	97529	4165	Reach_479	1500	168	96.8	1.4E-02	1.0E+03	3.5E+01		12.9	3.5E-06	1.1E-07	3.5E-07				14%	-7.5	-8.4	-10.5
(4R,6R)-4-Hydroxy-2,2,6-trimethylcyclohexanone	700-220-3	99636-32-5	99636325	4212	Reach_4808	1501	89	-52.1	5.4E+03	2.0E+05	3.2E-01			1.1E-06	1.1E-07	3.5E-07				14%	-8.1	-8.4	-10.3
3-(4-methyl-1H-imidazol-1-yl)-5-(trifluoromethyl)aniline	255-848-6	42487-72-9	42487729	2894	Reach_2751	1502	181	148.7	6.9E-05	1.9E+03	2.5E+00		10	3.5E-06	3.5E-07	3.5E-06				14%	-7.7	-8.4	-10.4
erythromycin	204-040-1	114-07-8	114078	336	Reach_933	1503	734	349.8	2.8E-23	2.2E+00	3.0E+02	12.7	5	2.7E-07	1.1E-07	3.5E-07				17%	-7.7	-8.4	-10.1
sodium 2-(2-dodecyloxyethoxy)ethyl sulphate	221-416-0	3088-31-1	3088311	5836	Reach_1914	1504	376	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.1	-8.4	-10.1
N-bromosuccinimide	204-877-2	128-08-5	128085	1815	Reach_1106	1505	178	121.0	9.2E-04	1.3E+05	6.5E-02			3.5E-06	3.5E-07	1.1E-06				14%	-7.4	-8.4	-10.6
3-(trimethoxysilyl)propiononitrile	224-207-2	4246-51-9	4246519	2893	Reach_2022	1506	220	92.6	2.9E-02	1.0E+06	3.5E-02			1.1E-06	1.1E-07	3.5E-07				16%	-8.7	-8.4	-10.1
trimethoxyvinylsilane	220-449-8	2768-02-7	2768027	1255	Reach_1864	1507	148	-48.8	2.1E+03	1.4E+04	4.8E-01			3.5E-06	3.5E-07	1.1E-06				14%	-8.7	-8.4	-10.3
cetrimonium bromide	200-311-3	57-09-0	57090	1223	Reach_36	1508	364	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.1	-8.4	-10.1
4,4'-methylene bis(dibutyldithiocarbamate)	233-593-1	10254-57-6	10254576	1344	Reach_2285	1509	423	202.6	8.5E-08	3.9E-03	5.4E+06		15.4	3.5E-07	3.5E-08	3.5E-07				16%	-8.0	-8.4	-10.2
3,3'-[(2-chloro-5-methyl-p-phenylene)bis[imino(1-acetyl-2-oxo	941-126-4	1499193-66-6	1499193666	5706	Reach_5178	1510	865	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.1	-8.4	-10.1
methyl decanoate	203-766-6	110-42-9	110429	1520	Reach_813	1511	186	1.7	1.4E+01	1.7E+01	2.0E+04			3.5E-07	3.5E-08	1.1E-07				20%	-8.7	-8.4	-10.4
4,4',4''-(1-methylpropanyl-3-ylidene)tris[6-tert-butyl-m-cresol]	217-420-7	1843-03-4	1843034	2190	Reach_1724	1512	545	273.8	2.1E-13	1.8E-07	5.0E+12	10.3		1.1E-06	3.5E-08	1.1E-07				24%	-8.6	-8.4	-8.8
potassium sodium hydrogen 7-[(2-acetamido-4-[(4-ammonio-5	283-810-9	84713-17-7	84713177	3874	Reach_2977	1513	150	39.0	1.1E+00	2.0E+04	4.4E+01									18%	-8.1	-8.4	-10.1
tert-butyl (6S)-6-[4-(7-{2-[(1R,3S,4S)-2-(tert-butoxycarbonyl)-2-	601-507-5	118135-28-7	118135287	1666	Reach_4092	1514	247	74.1	1.2E-01	3.2E-03	1.2E+05									18%	-8.1	-8.4	-10.1
sodium hydrogen 3-{[4-({4-[(2-aminopropyl)amino]-6-chloro-1,	617-708-6	85390-94-9	85390949	3886	Reach_4472	1515	489	214.2	1.1E-10	1.4E-01	4.4E+04									18%	-8.1	-8.4	-10.1
2-[(1R,3S,4S)-2-azabicyclo[2.2.1]hept-3-yl]-5-(7-{2-[(6S)-5-azas	696-357-0	1182822-31-6	1182822316	1667	Reach_4715	1516	279	108.4	9.4E-04	1.3E+01	2.2E+04									18%	-8.1	-8.4	-10.1
disodium [7-amino-4-(hydroxy-kO)-3-[(2-{[2-(hydroxy-kO)-5-su	220-098-0	2627-86-3	2627863	2461	Reach_1848	1517	121	-0.1	7.2E+01	3.7E+03	3.1E+01									18%	-8.1	-8.4	-10.1
trisodium [2-[[α-[(3-amino-2-hydroxy-5-sulphophenyl)azo]ben	204-376-9	120-20-7	120207	1706	Reach_991	1518	181	68.1	3.5E-01	3.4E+03	9.5E+00									18%	-8.1	-8.4	-10.1
trisodium 7-[[4-[(4-aminophenyl)azo]phenyl]azo]naphthalene-	617-345-3	82543-14-4	82543144	3827	Reach_4453	1519	401	192.4	8.9E-09	5.4E+00	8.9E+03									18%	-8.1	-8.4	-10.1
benzyl benzoate	204-402-9	120-51-4	120514	359	Reach_996	1520	212	70.8	7.4E-02	7.3E+01	3.5E+03			5.8E-07	1.1E-07	3.5E-07				16%	-8.6	-8.4	-10.2
Trisodium 2-[(E)-(6-amino-1-hydroxy-3-sulfonato-2-naphthyl)d	917-818-7	73344-75-9	73344759	3620	Reach_5084	1521	193	81.7	1.1E-01	1.2E+04	3.7E+01									18%	-8.1	-8.4	-10.1
617-589-0	615-749-4	72291-30-6	72291306	3601	Reach_4416	1522	127	-4.1	7.5E+01	4.6E+04	2.5E+00									18%	-8.1	-8.4	-10.1
Trisodium 2-[(E)-(6-amino-1-hydroxy-3-sulfonato-2-naphthyl)d	607-929-6	26391-06-0	26391060	2467	Reach_4253	1523	140	60.6	4.7E-01	2.6E+04	5.6E+00									18%	-8.1	-8.4	-10.1
805-364-1	302-748-6	94133-84-3	94133843	6088	Reach_3006	1524	201	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.1	-8.4	-10.1
Trisodium 2-[(6-amino-1-hydroxy-3-sulfonato-2-naphthyl)diaze	260-591-8	57144-06-6	57144066	3226	Reach_2824	1525	300	136.9	6.4E-04	5.3E+00	3.9E+03									18%	-8.1	-8.4	-10.1
N,N'-diisopropylethane-1,2-diaminium bis[(2R,3Z,5R)-3-(2-hydr	212-658-8	838-88-0	838880	3851	Reach_1563	1526	226	142.5	1.2E-04	5.8E+01	1.9E+03									18%	-8.1	-8.4	-10.1
disodium 5-amino-4-hydroxy-3-[(2-hydroxy-5-nitrophenyl)azo]	210-789-5	623-36-9	623369	3366	Reach_1449	1527	98	-64.4	9.9E+02	1.3E+04	4.4E+01									18%	-8.1	-8.4	-10.1
(4S,4aS,5aR,12aS)-9-amino-4,7-bis(dimethylamino)-3,10,12,12	214-868-5	1203-17-4	1203174	1709	Reach_1673	1528	188	40.9	4.4E+00	2.9E+00	4.3E+05									18%	-8.1	-8.4	-10.1
disodium 3-[[2-(acetylamino)-4-aminophenyl]azo]naphthalene	615-309-1	7159-96-8	7159968	3585	Reach_4414	1529	181	83.2	2.7E-02	5.7E+03	2.6E+01									18%	-8.1	-8.4	-10.1
601-093-6	601-093-6	111453-32-8	111453328	1548	Reach_4078	1530	632	295.4	1.3E-17	2.7E-01	9.1E+00	1.69		1.1E-06	3.5E-07	1.1E-06				14%	-7.4	-8.4	-10.3
Sodium hydrogen 4-amino-2-{[1-ethyl-2-hydroxy-4-methyl-6-o	225-472-7	4866-00-6	4866006	2975	Reach_2065	1531	126	102.1	9.5E-02	7.6E+04	1.8E-01									18%	-8.1	-8.4	-10.1
613-004-8	254-301-9	39118-50-8	39118508	2835	Reach_2723	1532	196	19.9	2.8E+00	5.5E+04	2.8E-01									18%	-8.1	-8.4	-10.1
2-[2-(dimethylamino)ethoxy]ethanol	216-940-1	1704-62-7	1704627	2119	Reach_1710	1533	133	1.7	9.3E+00	1.0E+06	6.2E-02	14.9	5.26	1.1E-06	3.5E-07	1.1E-06				14%	-8.0	-8.4	-10.5
1,3-Thiazol-5-ylmethyl [(2R,5R)-5-amino-1,6-diphenylhexan-2-y	700-597-4	1215841-86-3	1215841863	1729	Reach_4945	1534	346	247.7	3.1E-14	1.5E+05	8.1E-04									18%	-8.1	-8.4	-10.1
sodium hydrogen 2-({4-[(2-aminopropyl)amino]-6-fluoro-1,3,5-	619-846-2	123989-28-6	123989286	1779	Reach_4549	1535	211	64.4	9.7E-03	1.9E+02	6.9E+03									18%	-8.1	-8.4	-10.1
Ammonium (3R,5R)-3,5-dihydroxy-7-[(1S,2S,6S,8S,8aR)-6-hydr	201-379-7	81-83-4	81834	3815	Reach_279	1536	197	210.4	5.1E-08	2.0E+02	9.8E+01									18%	-8.1	-8.4	-10.1
barium bis(2-ethylhexanoate)	941-128-5	1499193-67-7	1499193677	5707	Reach_5179	1537	721	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.1	-8.4	-10.1
2-{2-[4-(dibenzo[b,f][1,4]thiazepin-11-yl)piperazin-1-yl]ethoxy}	602-964-3	123989-29-7	123989297	1780	Reach_4108	1538	209	62.6	2.8E-01	6.3E+00	1.0E+04									18%	-8.1	-8.4	-10.1
Sodium 2-[(E)-(4-ammonio-2,5-dimethylphenyl)diazenyl]benze	688-501-6	21700-31-2	21700312	2303	Reach_4645	1539	216	-9.1	1.3E+02	7.3E+01	4.0E+03									18%	-8.1	-8.4	-10.1
3,3'-dichloro[1,1'-biphenyl]-4,4'-bis(diazonium) dichloride	212-946-3	885-82-5	885825	3960	Reach_1584	1540	215	138.9	7.4E-05	2.7E+01	4.7E+03									18%	-8.1	-8.4	-10.1
613-879-6	279-356-6	79953-85-8	79953858	6406	Reach_2958	1541	1229	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.1	-8.4	-10.1
3-ethoxypropylamine	211-951-8	719-80-2	719802	3596	Reach_1523	1542	230	69.5	2.7E-02	3.6E+00	4.0E+03			1.1E-06	1.1E-07	3.5E-07				16%	-8.7	-8.4	-9.8
α,α-diphenylpiperidine-4-methanol hydrochloride	605-954-7	181997-71-7	181997717	2173	Reach_4185	1543	215	77.9	7.1E-02	5.6E+01	3.0E+03									18%	-8.1	-8.4	-10.1
608-782-0	248-576-4	27619-89-2	27619892	2513	Reach_2610	1544	447	30.9	3.4E+01	6.3E-01	2.0E+06									18%	-8.1	-8.4	-10.1
pentasodium 2-{[8-({4-fluoro-6-[(4-{[2-(sulfonatooxy)ethyl]sulf	612-957-7	62211-93-2	62211932	5954	Reach_4377	1545	520	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.1	-8.4	-10.1
octocrilene	228-250-8	6197-30-4	6197304	3360	Reach_2157	1546	361	180.8	4.2E-07	3.5E-02	7.6E+06			1.1E-06	1.1E-07	3.5E-07				21%	-8.0	-8.4	-9.6
Dibenzo[b,f][1,4]thiazepin-11-amine hydrochloride (1:1)	602-965-9	123989-31-1	123989311	1781	Reach_4109	1547	197	43.3	5.3E-02	2.5E+02	2.5E+03									18%	-8.1	-8.4	-10.1
diammonium propylenebis(dithiocarbamate)	215-863-0	1435-71-8	1435718	1968	Reach_1680	1548	257	156.5	8.9E-06	9.5E+00	1.9E+05									18%	-8.1	-8.4	-10.1
sodium 3-hydroxy-2-naphthoate	223-423-4	3886-69-9	3886699	2827	Reach_1997	1549	121	-0.1	7.2E+01	3.7E+03	3.1E+01									18%	-8.1	-8.4	-10.1
611-210-2	248-479-7	27472-21-5	27472215	2509	Reach_2606	1550	205	94.6	1.4E-02	1.6E+02	1.5E+02									18%	-8.1	-8.4	-10.1
nickel(2+) propionate	220-612-3	2835-68-9	2835689	2527	Reach_1873	1551	136	118.6	7.1E-04	4.2E+03	6.6E-01									18%	-8.1	-8.4	-10.1
2-amino-2-phenylbutyrate sodium	606-239-2	19130-96-2	19130962	2222	Reach_4199	1552	163	129.2	7.2E-06	8.8E+05	1.7E-03									18%	-8.1	-8.4	-10.1

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
N-tert-butylglycyl chloride hydrochloride (1:1)	603-266-1	128286-13-5	128286135	1818	Reach_4113	1553	752	282.7	6.7E-13	1.7E-03	9.3E+02									18%	-8.1	-8.4	-10.1
1-fluoro-4-nitrobenzene	206-502-8	350-46-9	350469	611	Reach_1242	1554	141	25.4	3.7E+01	1.4E+03	1.0E+02			2.2E-09	1.1E-07	3.5E-07				23%	-8.7	-8.4	-9.7
sodium 2-hexyloxyethanolate	206-566-7	354-64-3	354643	2738	Reach_1249	1555	246	-89.4	1.5E+05	3.5E+03	9.3E+02									18%	-8.1	-8.4	-10.1
612-957-7	679-514-8	154279-60-4	154279604	2034	Reach_4620	1556	323	121.3	3.9E-04	9.1E-04	1.0E+07									18%	-8.1	-8.4	-10.1
sodium 4-aminobenzoate	217-385-8	1830-54-2	1830542	2178	Reach_1723	1557	174	-46.6	3.5E+01	8.2E+04	7.1E-02									18%	-8.1	-8.4	-10.1
sodium anthranilate	605-991-9	183322-16-9	183322169	2184	Reach_4187	1558	298	122.6	8.1E-04	1.9E+02	2.6E+01									18%	-8.1	-8.4	-10.1
602-891-7	602-891-7	122731-59-3	122731593	1758	Reach_4107	1559	716	294.8	9.7E-14	1.7E-02	3.6E+02	1.68		1.1E-06	1.1E-07	1.1E-06				14%	-7.7	-8.4	-10.3
sodium taurinate	219-265-0	2398-81-4	2398814	2363	Reach_1793	1560	139	118.2	2.0E-04	5.4E+04	3.5E-02									18%	-8.1	-8.4	-10.1
ethyl glycinate hydrochloride	607-358-2	24338-09-8	24338098	2388	Reach_4239	1561	256	36.2	6.1E-01	6.7E-01	2.7E+06									18%	-8.1	-8.4	-10.1
cyclohexane-1,3-dione, monosodium salt	606-440-5	201214-53-1	201214531	2251	Reach_4209	1562	349	177.1	6.1E-06	1.6E+02	1.0E+02									18%	-8.1	-8.4	-10.1
anisaldehyde	204-602-6	123-11-5	123115	1763	Reach_1039	1563	136	12.8	4.0E+00	4.8E+03	6.2E+01			1.1E-06	3.5E-07	1.1E-06				14%	-8.7	-8.4	-10.3
sodium β-alaninate	692-511-6	63661-82-5	63661825	3416	Reach_4675	1564	487	349.8	6.1E-24	2.1E-05	2.1E-01									18%	-8.1	-8.4	-10.1
O,O-dimethyl phosphorochloridothioate	219-754-9	2524-03-0	2524030	2424	Reach_1828	1565	161	-97.6	4.0E+02	3.2E+03	2.5E+01			1.1E-06	1.1E-07	1.1E-06				15%	-8.7	-8.4	-10.0
N-methylacetamide	229-542-8	6600-31-3	6600313	3458	Reach_2195	1566	320	141.7	2.3E-04	3.2E+01	2.3E+04	0	0	1.1E-06	3.5E-07	1.1E-06				16%	-8.1	-8.4	-10.3
bis(2,4-dichlorophenyl) carbonate	247-748-6	26496-99-1	26496991	2471	Reach_2584	1567	352	137.0	6.5E-05	6.7E-02	6.0E+05			1.1E-07	3.5E-09	1.1E-08				22%	-8.6	-8.4	-9.7
but-2-ene-1,4-diol	212-472-7	821-06-7	821067	3818	Reach_1553	1568	214	-15.8	3.0E+01	8.9E+02	6.0E+02			3.5E-07	3.5E-08	1.1E-07				14%	-7.7	-8.4	-10.4
618-109-2	208-844-3	543-49-7	543497	3139	Reach_1350	1569	116	-39.3	1.1E+02	4.9E+03	1.7E+02			1.1E-06	3.5E-07	1.1E-06				17%	-8.6	-8.4	-9.9
608-991-7	259-197-9	54527-65-0	54527650	3147	Reach_2800	1570	249	98.1	6.1E-03	1.2E+02	5.1E+00			1.1E-06	1.1E-07	3.5E-07				17%	-8.6	-8.4	-9.9
[3-(2,3-epoxypropoxy)propyl]triethoxysilane	220-011-6	2602-34-8	2602348	2449	Reach_1843	1571	278	77.7	7.7E-02	6.8E+02	3.6E+00			3.5E-07	1.1E-07	3.5E-07				16%	-8.6	-8.4	-10.3
Heptan-2-yl [(5-chloroquinolin-8-yl)oxy]acetate	619-447-3	99607-70-2	99607702	1089	Reach_4521	1572	336	154.9	1.6E-04	4.8E-01	1.9E+05		11	1.7E-07	1.1E-07	1.1E-06				18%	-8.0	-8.4	-10.1
3-methylbutan-1-ol	204-633-5	123-51-3	123513	394	Reach_1051	1573	88	-61.5	5.1E+02	2.7E+04	1.8E+01	15.9		3.8E-07	1.1E-06	3.5E-06				16%	-8.7	-8.4	-9.7
1,3,5-tris[[4-tert-butyl-3-hydroxy-2,6-xylyl]methyl]-1,3,5-triazin	254-996-9	40601-76-1	40601761	2859	Reach_2731	1574	700	349.8	8.5E-25	8.2E-08	1.9E+15	11.5	14.2	3.5E-07	3.5E-08	1.1E-07				24%	-8.7	-8.4	-7.5
triethoxy(vinyl)silane	201-081-7	78-08-0	78080	3746	Reach_193	1575	190	-12.8	9.6E+01		1.4E+01			1.1E-06	3.5E-07	1.1E-06				14%	-8.7	-8.4	-10.2
dimethyl 2,5-dioxocyclohexane-1,4-dicarboxylate	202-676-4	98-52-2	98522	1072	Reach_509	1576	156	4.3	1.4E+00	8.1E+01	2.6E+03	16		2.6E-07	1.1E-07	3.5E-07				14%	-7.6	-8.4	-10.6
1-[4-(1,1-dimethylethyl)phenyl]-3-(4-methoxyphenyl)propane-	274-581-6	70356-09-1	70356091	3560	Reach_2917	1577	310	155.1	1.8E-04	1.8E+00	3.2E+04	8.15		1.1E-06	1.1E-07	3.5E-07				16%	-8.6	-8.4	-10.2
endo-8-isopropyl-8-azabicyclo[3.2.1]octan-3-ol	640-387-9	61477-40-5	61477405	3335	Reach_4608	1578	89	-14.7	1.0E+02	8.6E+05	2.0E-01	15.3	4.1	3.5E-06	1.1E-06	3.5E-06				14%	-8.4	-8.4	-10.4
amoxicillin	265-634-4	65212-77-3	65212773	5973	Reach_2871	1579	545	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				17%	-7.7	-8.4	-10.1
α-acetyl-γ-butyrolactone	700-856-1	1247119-31-8	1247119318	5639	Reach_5015	1580	341	0.0												14%	-8.5	-8.4	-10.5
succinonitrile	248-003-8	26787-78-0	26787780	574	Reach_2594	1581	365	329.9	6.3E-15	2.1E+04	9.3E+00			2.1E-07	3.5E-07	1.1E-06				16%	-8.0	-8.4	-10.3
N-[(tert-butoxy)carbonyl]-L-valine	250-196-9	30433-91-1	30433911	2597	Reach_2647	1582	127	32.0	2.0E+01	1.1E+03	2.4E+01			1.1E-06	3.5E-08	1.1E-07				14%	-7.8	-8.4	-10.4
4,4'-methylenebis[N,N-bis(2,3-epoxypropyl)aniline]	249-204-3	28768-32-3	28768323	2543	Reach_2623	1583	423	217.7	1.7E-08	4.7E+00	3.4E+02		10.1	1.1E-06	3.5E-08	1.1E-07				14%	-7.6	-8.4	-10.5
4-amino-6-chlorotoluene-3-sulphonic acid	201-837-6	88-51-7	88517	3959	Reach_326	1584	222	149.6	2.1E-06	1.1E+03	1.3E-01	-1.16	12.2	1.1E-06	3.5E-07	1.1E-06				14%	-7.2	-8.4	-10.4
D-gluconic acid, compound with N,N''-bis(4-chlorophenyl)-3,12	203-157-5	103-90-2	103902	165	Reach_616	1585	151	119.9	2.6E-04	8.1E+03	1.9E+00									18%	-8.1	-8.4	-10.1
691-232-7	691-232-7	474266-68-7	474266687	5894	Reach_4665	1586	204	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.1	-8.4	-10.1
acid D,L-aspart	216-431-4	1583-59-1	1583591	2061	Reach_1697	1587	158	10.4	1.4E+02	7.3E+02	4.3E+03			1.1E-06	3.5E-07	1.1E-06				14%	-7.1	-8.4	-10.5
600-709-0	246-014-2	24085-08-3	24085083	5789	Reach_2538	1588	364	0.0												14%	-7.7	-8.4	-10.4
608-880-3	606-067-8	18595-18-1	18595181	2199	Reach_4191	1589	165	64.9	3.2E-01	3.5E+03	7.1E+01			3.5E-06	3.5E-07	1.1E-06				14%	-7.8	-8.4	-10.4
2'-ethoxy-3-hydroxy-2-naphthanilide	202-185-5	92-74-0	92740	4048	Reach_391	1590	307	221.7	1.1E-09	5.2E+00	3.0E+04	10.2		3.5E-07	3.5E-08	1.1E-07				18%	-7.7	-8.4	-10.1
demeclocycline hydrochloride	200-592-2	64-73-3	64733	5969	Reach_74	1591	501	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.1	-8.4	-10.1
D-(-)-α-phenylglycine	200-752-1	71-41-0	71410	820	Reach_102	1592	88	-50.0	3.5E+02	3.0E+04	2.1E+01	15.9		4.0E-06	1.1E-06	3.5E-06				14%	-7.1	-8.4	-10.5
1,4-dioxane	204-661-8	123-91-1	123911	16	Reach_1060	1593	88	-63.6	5.4E+03	4.4E+04	4.8E-01			3.7E-09	1.1E-07	3.5E-07				23%	-8.7	-8.4	-9.9
dibenzoyl-L-tartaric acid monohydrate	242-040-3	18156-74-6	18156746	2169	Reach_2453	1594	140	29.0	8.0E+00	1.7E+03	2.4E+02			3.5E-07	3.5E-08	1.1E-07				14%	-7.8	-8.4	-10.3
6-Fluorochromane-2-carboxylic acid	610-555-6	50650-75-4	50650754	3013	Reach_4332	1595	222	62.2	3.4E-02	2.1E+00	1.3E+04			3.5E-06	3.5E-07	1.1E-06				14%	-7.8	-8.4	-10.4
603-772-2	247-362-8	25953-19-9	25953199	2448	Reach_2572	1596	455	333.0	2.0E-16	2.6E+01	2.5E-03	2.6		1.1E-07	1.1E-07	3.5E-07				15%	-7.7	-8.4	-10.4
4-tert-butylcyclohexanol	203-137-6	103-71-9	103719	1378	Reach_612	1597	119	-37.3	2.9E+02	4.0E+04	3.9E+02			1.1E-06	3.5E-07	1.1E-06				17%	-8.7	-8.4	-9.7
cyclohexane-1,3-dione	207-980-0	504-02-9	504029	3005	Reach_1303	1598	112	21.5	5.6E+00	4.1E+05	2.7E+00	5.4		1.1E-06	3.5E-07	1.1E-06				14%	-7.6	-8.4	-10.4
isobutyric acid	201-195-7	79-31-2	79312	919	Reach_239	1599	88	-8.3	4.4E+02	1.1E+05	1.0E+01	4.9		4.7E-06	3.5E-07	1.1E-06				14%	-8.1	-8.4	-10.4
2-chloro-3-(dimethylamino)-N,N-dimethylprop-2-en-1-iminium	280-445-7	83411-71-6	83411716	3845	Reach_2966	1600	290	79.4	1.7E-04	4.5E+00	2.2E+05									18%	-8.1	-8.4	-10.1
N-(2-benzoyl-4-chlorophenyl)cyclopropanecarboxamide	200-453-6	60-09-3	60093	746	Reach_54	1601	197	93.6	7.0E-04	6.0E+02	1.5E+03	0	11	1.5E-08	3.5E-07	1.1E-06				19%	-8.1	-8.4	-10.0
607-327-3	609-368-2	3724-43-4	3724434	5864	Reach_4300	1602	128	0.0												14%	-8.7	-8.4	-10.4
4-methylanisole	203-253-7	104-93-8	104938	1403	Reach_634	1603	122	-23.0	1.6E+02	3.6E+02	4.2E+02			3.5E-06	3.5E-07	1.1E-06				15%	-8.7	-8.4	-10.4
1,1,1-trifluoroethane	206-996-5	420-46-2	420462	2887	Reach_1269	1604	84	-151.7	9.3E+05	3.2E+04	5.5E+01			3.5E-07	1.1E-07	3.5E-07				22%	-8.8	-8.4	-10.7
2-ethoxy-1-methylethyl acetate	259-370-9	54839-24-6	54839246	3154	Reach_2802	1605	146	-38.2	3.7E+02	1.6E+04	1.0E+01			1.1E-06	3.5E-07	1.1E-06				14%	-8.7	-8.4	-9.9
bis(2-methylisouronium) sulphate	245-642-4	23410-40-4	23410404	2351	Reach_2531	1606	220	55.9	1.1E+00	4.0E+04	1.0E+00									18%	-8.1	-8.4	-10.1
α-chloro-4-fluoroacetophenone	218-377-7	2136-89-2	2136892	2291	Reach_1761	1607	230	40.5	1.5E+00	7.7E+00	3.5E+04			1.1E-07	1.1E-08	3.5E-08				15%	-8.7	-8.4	-10.1
3,3'-oxybis(ethyleneoxy)bis(propylamine)	219-764-3	2526-62-7	2526627	2427	Reach_1830	1608	175	21.3	1.2E+01	6.4E+03	6.9E-02		0	3.5E-07	1.1E-07	3.5E-07				14%	-7.4	-8.4	-10.6
610-491-9	212-726-7	859-18-7	859187	1237	Reach_1567	1609	443	0.0												15%	-8.0	-8.4	-10.4
12-aminododecanoic acid	204-251-9	118-45-6	118456	1670	Reach_963	1610	183	50.8	4.4E-01	8.5E+01	5.1E+02	0	0	1.1E-06	1.1E-07	3.5E-07				14%	-7.3	-8.4	-10.5
3-aminobenzenesulphonic acid	204-473-6	121-47-1	121471	1728	Reach_1015	1611	173	128.1	2.7E-05	3.9E+04	8.3E-03	-0.39	10.3	1.1E-06	1.1E-07	1.1E-06				14%	-7.4	-8.4	-10.6
dibutyltin di(acetate)	213-928-8	1067-33-0	1067330	199	Reach_1639	1612	351	55.3	4.0E-01	0.0E+00	6.5E+00			2.2E-09	3.5E-07	1.1E-06				23%	-8.3	-8.4	-9.4
2,2-dimethylpropan-1-ol, tribromo derivative	253-057-0	36483-57-5	36483575	2768	Reach_2700	1613	325	74.3	1.6E-02	9.8E+01	7.1E+02	14.5		1.1E-06	3.5E-07	1.1E-06				15%	-8.7	-8.4	-10.3
3-methyl-1-phenyl-5-pyrazolone	216-319-5	1558-33-4	1558334	2045	Reach_1690	1614	164	-55.8	1.9E+03		3.2E+02			1.1E-07	1.1E-08	3.5E-08				15%	-7.7	-8.4	-10.4
tetradecyl methacrylate	219-835-9	2549-53-3	2549533	2435	Reach_1835	1615	282	54.7	2.4E-02	1.8E-02	4.6E+07			1.1E-06	1.1E-07	3.5E-07				22%	-8.5	-8.4	-10.4
616-785-3	231-001-6	7400-27-3	7400273	6020	Reach_2249	1616	125	0.0												15%	-7.7	-8.4	-10.4
but-3-en-3-olide	211-617-1	674-82-8	674828	3493	Reach_1494	1617	84	-35.6	1.6E+03	9.3E+04	4.1E-01			3.5E-06	3.5E-07	1.1E-06				14%	-8.7	-8.4	-10.1
piperidine	203-813-0	110-89-4	110894	289	Reach_836	1618	85	-24.7	3.9E+03	3.2E+05	1.5E+01		3	5.3E-07	1.1E-07	3.5E-07				15%	-8.7	-8.4	-9.8
isovaleraldehyde	209-691-5	590-86-3	590863	733	Reach_1389	1619	86	-79.3	6.9E+03	1.9E+04	1.7E+01			3.8E-07	1.1E-06	3.5E-06				17%	-8.7	-8.4	-10.1
bis(2-ethylhexyl) peroxydicarbonate	240-282-4	16111-62-9	16111629	2079	Reach_2413	1620	346	63.6	3.0E-04	1.2E+00	9.3E+06			3.5E-07	3.5E-08	1.1E-07				22%	-8.1	-8.4	-9.6
endo-(±)-8-aza-8-isopropylbicyclo[3.2.1]oct-3-yl (hydroxymethy	606-548-2	204254-84-2	204254842	2263	Reach_4211	1621	320	151.9	6.3E-05	2.0E+03	8.7E+00			3.5E-06	3.5E-07	1.1E-06				15%	-7.6	-8.5	-10.3
4-tert-butylbenzaldehyde	213-367-9	939-97-9	939979	4095	Reach_1613	1622	162	25.0	6.1E+00	5.5E+01	4.2E+03			1.1E-06	1.1E-07	3.5E-07				16%	-8.7	-8.5	-10.0
hexahydro-1,3,5-tris(1-oxoallyl)-1,3,5-triazine	213-501-6	959-52-4	959524	4138	Reach_1619	1623	249	163.7	2.2E-05	1.1E+04	2.2E-03			3.5E-06	1.1E-07	3.5E-07				14%	-7.4	-8.5	-10.8
dimethyl isophthalate	215-951-9	1459-93-4	1459934	1990	Reach_1685	1624	194	-22.7	2.7E-01	1.9E+03	4.6E+01			1.1E-06	1.1E-07	3.5E-07				14%	-8.7	-8.5	-10.4
trimethyl phosphite	204-471-5	121-45-9	121459	1727	Reach_1014	1625	124	-57.6	3.0E+03	8.7E+04	1.9E-01			1.1E-06	1.1E-07	1.1E-06				14%	-8.7	-8.5	-9.9
hexadecyldimethylamine	203-997-2	112-69-6	112696	1598	Reach_919	1626	270	62.8	3.8E-02	1.3E-02	2.6E+07		3.9	1.1E-06	1.1E-07	3.5E-07				22%	-8.5	-8.5	-10.7
617-346-9	700-272-7	754186-36-2	754186362	6026	Reach_4832	1627	405	0.0												14%	-7.6	-8.5	-10.3

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
2-amino-6-fluorobenzonitrile	204-485-1	121-60-8	121608	1730	Reach_1017	1628	234	166.4	4.5E-05	4.5E+03	1.1E+02		15.8	1.1E-06	1.1E-07	3.5E-07				14%	-8.7	-8.5	-10.3
5-chloro-o-toluidine	258-907-4	53994-69-7	53994697	3116	Reach_2796	1629	235	299.0	7.5E-08	5.0E+03	3.1E-01		7.25	3.5E-07	1.1E-07	3.5E-07				14%	-7.9	-8.5	-10.4
606-722-8	212-786-4	869-24-9	869249	6071	Reach_1576	1630	172	0.0												19%	-7.6	-8.5	-10.0
N-[(1,1,3,3-tetramethylbutyl)phenyl]naphthalen-1-amine	257-406-8	51772-35-1	51772351	3046	Reach_2774	1631	332	155.4	1.5E-05	5.5E-03	1.7E+08		13.2	3.5E-07	1.1E-08	3.5E-08				16%	-8.1	-8.5	-10.3
1-(2,2-difluoro-1,3-benzodioxol-5-yl)cyclopropanecarboxylic ac	688-133-6	338-65-8	338658	2688	Reach_4641	1632	101	-121.4	9.5E+04	5.4E+03	2.5E+01			1.1E-07	1.1E-08	3.5E-08				14%	-7.9	-8.5	-10.4
octan-2-ol	204-667-0	123-96-6	123966	399	Reach_1063	1633	130	-27.5	3.2E+01	1.8E+03	5.4E+02	16		4.2E-07	1.1E-07	3.5E-07				16%	-8.7	-8.5	-9.8
hexa-2,4-dienoic acid	208-482-6	530-48-3	530483	3084	Reach_1326	1634	180	21.0	8.4E-01	1.0E+01	7.2E+03			1.1E-06	1.1E-07	3.5E-07				14%	-7.8	-8.5	-10.4
2-tert-butyl-p-cresol	219-314-6	2409-55-4	2409554	2373	Reach_1800	1635	164	51.9	1.7E+00	5.3E+02	9.3E+03	10.8		3.5E-06	3.5E-07	1.1E-06				15%	-8.7	-8.5	-10.3
prop-2-yn-1-ol	203-471-2	107-19-7	107197	214	Reach_698	1636	56	-49.0	1.3E+03	3.7E+05	3.8E-01	13.6		2.9E-06	1.1E-06	3.5E-06				14%	-8.7	-8.5	-10.2
4-chloro-o-xylene	210-248-3	611-06-3	611063	755	Reach_1417	1637	192	65.7	1.9E+00	7.5E+01	1.3E+03			2.3E-09	1.1E-08	3.5E-08				21%	-8.8	-8.5	-10.7
4-chloro-α,α,α-trifluoro-o-toluidine	210-856-9	624-65-7	624657	3372	Reach_1454	1638	75	-72.1	2.8E+04	1.1E+04	2.0E+01			1.1E-07	1.1E-08	3.5E-08				14%	-8.3	-8.5	-10.4
biphenyl	202-163-5	92-52-4	92524	1012	Reach_385	1639	154	25.1	1.0E+00	5.0E+00	5.8E+03			9.1E-07	1.1E-08	3.5E-08				16%	-8.7	-8.5	-10.1
hexafluoropropene	204-127-4	116-15-4	116154	1646	Reach_952	1640	150	-152.7	5.9E+05	1.1E+00	1.3E+02			3.5E-08	1.1E-08	3.5E-08				23%	-8.8	-8.5	-11.2
trichloro(hexadecyl)silane	227-575-2	5894-60-0	5894600	3260	Reach_2142	1641	360	89.6	7.3E-03	2.6E-01	2.3E+09			1.1E-06	1.1E-07	3.5E-07				23%	-8.3	-8.5	-9.1
α-hydroxy-β,β-dimethyl-γ-butyrolactone	209-963-3	599-04-2	599042	3296	Reach_1408	1642	130	31.2	5.5E-02	1.8E+05	1.1E-01	12.6		3.5E-06	3.5E-07	1.1E-06				14%	-7.5	-8.5	-10.6
2-oxo-2-[(4aS,4bS,5aS,6aS,6bS,9aR,10aS,10bS)-4a,6a,8,8-tetra	607-542-2	25092-32-4	25092324	2414	Reach_4243	1643	457	215.5	2.4E-08	8.8E+00	1.1E+03			1.1E-06	1.1E-07	3.5E-07				15%	-7.7	-8.5	-10.3
bis(2-hydroxyethyl) (6H-dibenz[c,e][1,2]oxaphosphorin-6-ylme	264-313-6	63562-34-5	63562345	3405	Reach_2860	1644	434	90.3	8.1E-09	1.3E+02	2.1E+00	13.9		3.5E-07	3.5E-08	1.1E-07				16%	-7.4	-8.5	-10.4
O-(1-chloroethyl) S-methyl carbonothioate	700-190-1	91507-67-4	91507674	4016	Reach_4799	1645	155	-28.1	1.4E+02	2.1E+03	2.5E+01			1.1E-06	1.1E-07	1.1E-06				15%	-8.7	-8.5	-10.0
4,6-diphenyl-1,3,5-triazin-2(1H)-one	222-374-6	3452-07-1	3452071	1261	Reach_1963	1646	281	50.4	5.5E-02	5.7E-05	1.1E+10			1.1E-06	1.1E-07	3.5E-07				15%	-7.7	-8.5	-10.3
sodium 1,4-diisotridecyl sulphonatosuccinate	619-547-7	211515-46-7	211515467	2284	Reach_4529	1647	231	52.6	1.0E+00	6.7E-02	4.3E+04									18%	-8.2	-8.5	-10.1
2-aminobenzene-1,4-disulphonic acid	202-669-6	98-44-2	98442	4185	Reach_507	1648	253	211.4	1.0E-10	2.5E+04	9.3E-04	-1.89	12	1.1E-06	1.1E-07	1.1E-06				14%	-7.2	-8.5	-10.5
1-ethylpiperazine	226-166-6	5308-25-8	5308258	3087	Reach_2096	1649	114	9.9	1.6E+02	7.2E+05	7.9E-01		5	3.5E-06	3.5E-07	1.1E-06				14%	-8.7	-8.5	-10.5
dipotassium hydrogen 7-aminonaphthalene-1,3,6-trisulphonat	284-333-9	84852-23-3	84852233	6054	Reach_2980	1650	460	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.2	-8.5	-10.1
4-methylpent-3-en-2-one	205-502-5	141-79-7	141797	1942	Reach_1169	1651	98	-64.4	1.6E+03	7.4E+03	2.3E+01			1.1E-06	3.5E-07	1.1E-06				15%	-8.7	-8.5	-10.1
2-methyl-3-phenylpropanol	221-639-3	3173-53-3	3173533	2630	Reach_1925	1652	125	-8.1	1.9E+02	1.3E+04	1.1E+03			1.1E-06	3.5E-07	1.1E-06				15%	-8.7	-8.5	-10.4
phenylacetonitrile	609-997-2	42221-52-3	42221523	4319	Reach_4319	1653	278	93.2	3.5E-02	1.9E+00	1.0E+04			3.5E-08	1.1E-08	3.5E-08				16%	-8.7	-8.5	-9.9
609-997-2	617-843-0	86386-77-8	86386778	6063	Reach_4476	1654	333	0.0												22%	-8.8	-8.5	-9.7
7-hydroxycitronellal	203-518-7	107-75-5	107755	1468	Reach_714	1655	172	23.4	7.7E-01	2.8E+04	1.3E+02	16		1.1E-06	1.1E-07	3.5E-07				14%	-8.5	-8.5	-10.4
bornan-2-one	200-945-0	76-22-2	76222	872	Reach_175	1656	152	28.1	1.4E+00	1.0E+03	1.1E+03			4.8E-07	3.5E-07	1.1E-06				16%	-8.7	-8.5	-10.2
butan-2-one O,O',O''-(vinylsilylidyne)trioxime	218-747-8	2224-33-1	2224331	2325	Reach_1774	1657	313	12.3	2.9E-02	0.0E+00	1.5E+10			3.5E-07	1.1E-07	3.5E-07				24%	-8.6	-8.5	-9.6
4-methylmorpholine	203-640-0	109-02-4	109024	1493	Reach_769	1658	101	-29.0	2.5E+03	1.4E+06	4.5E-01		6.5	1.1E-06	1.1E-07	3.5E-07				14%	-8.7	-8.5	-10.3
Propan-2-yl [(4R,6R)-6-{2-[2-(4-fluorophenyl)-3-phenyl-4-(phen	700-243-9	1112262-71-1	1112262711	1543	Reach_4818	1659	641	344.6	3.0E-17	4.3E-06	1.0E+10	14.3	15.9	3.5E-07	3.5E-08	1.1E-07				16%	-7.9	-8.5	-10.2
1-benzyl-3-carboxylatopyridinium sodium chloride	268-692-9	68133-60-8	68133608	5993	Reach_2897	1660	272	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.2	-8.5	-10.1
flufenamic acid	939-996-5	689294-28-8	689294288	3532	Reach_5162	1661	681	349.8	3.9E-19	7.4E-02	1.4E+04	10.1		3.5E-07	1.1E-07	3.5E-07				14%	-7.9	-8.5	-10.4
2-ethylhexyl mercaptoacetate	231-626-4	7659-86-1	7659861	3721	Reach_2267	1662	204	16.4	1.1E+03	6.1E+01	4.8E+03	8		3.5E-06	3.5E-07	1.1E-06				18%	-8.8	-8.5	-11.6
N,N-dimethyltetradecylamine N-oxide	222-059-3	3332-27-2	3332272	2679	Reach_1949	1663	257	183.3	1.5E-06	5.2E-02	4.6E+05		9.2	1.1E-06	1.1E-07	3.5E-07				15%	-7.9	-8.5	-10.4
3,3'-thiodi(propionic acid)	203-841-3	111-17-1	111171	1539	Reach_846	1664	178	126.6	1.9E-03	6.9E+04	6.6E-01	3.97		3.5E-06	3.5E-07	1.1E-06				14%	-7.4	-8.5	-10.5
2-[(2-acetamido-6,9-dihydro-6-oxo-1H-purin-9-yl]methoxy]eth	236-307-3	13290-96-5	13290965	1862	Reach_2328	1665	239	76.9	2.5E-02	1.6E+02	3.0E+01			1.1E-06	1.1E-07	3.5E-07				14%	-7.2	-8.5	-10.5
Methyl 2-amino-3-chlorobenzoate	607-917-0	263355-39-1	263355391	2465	Reach_4252	1666	229	70.4	1.7E-01	2.2E+03	8.5E+02			1.1E-06	1.1E-07	1.1E-06				15%	-8.7	-8.5	-10.4
2-(3-(4-amino-9,10-dihydro-3-sulpho-9,10-dioxoanthracen-4-yl	219-949-9	2580-78-1	2580781	5799	Reach_1841	1667	627	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.2	-8.5	-10.1
(E)-1,4-dibromobut-2-ene	606-728-0	212322-56-0	212322560	2287	Reach_4214	1668	342	205.6	1.1E-07	9.4E+02	8.7E+00			1.1E-06	1.1E-07	3.5E-07				17%	-8.8	-8.5	-9.9
salicylonitrile	210-259-3	611-20-1	611201	3327	Reach_1420	1669	119	53.8	3.2E-01	1.5E+04	4.1E+01	6.9		1.1E-05	1.1E-06	3.5E-06				14%	-8.2	-8.5	-10.4
disodium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4-)-N	238-372-3	14402-88-1	14402881	5698	Reach_2365	1670	359	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.2	-8.5	-10.1
613-099-6	218-491-7	2163-00-0	2163000	2301	Reach_1768	1671	155	-28.5	3.9E+01	2.1E+02	6.3E+03			3.5E-07	3.5E-08	1.1E-07				18%	-8.2	-8.5	-10.2
2-(3-chlorophenyl)-2,4-dihydro-5-methyl-3H-pyrazol-3-one	216-544-9	1609-86-5	1609865	2078	Reach_1699	1672	99	-44.8	1.8E+03	1.5E+04	1.4E+02			1.1E-06	3.5E-07	1.1E-06				15%	-7.8	-8.5	-10.4
methyl trimethyl-3-[(1-oxododecyl)amino]propylammonium su	234-204-8	10595-49-0	10595490	5596	Reach_2300	1673	411	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.2	-8.5	-10.2
1-[2-(dimethylamino)-1-(4-methoxyphenyl)ethyl]cyclohexanol	608-782-0	32765-81-4	32765814	5844	Reach_4282	1674	303	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				21%	-8.2	-8.5	-9.8
glycine	200-272-2	56-40-6	56406	3197	Reach_27	1675	75	246.2	1.1E-05	1.8E+05	3.9E-04	2.3	4.2	3.5E-06	3.5E-07	1.1E-06				14%	-7.2	-8.5	-10.6
octylphosphonic acid	225-218-5	4724-48-5	4724485	2964	Reach_2060	1676	194	76.2	1.1E-04	1.6E+03	2.8E+02	2.6		1.1E-06	1.1E-07	3.5E-07				14%	-7.8	-8.5	-10.5
2-(2-phenoxyethoxy)ethanol	257-093-8	51263-08-2	51263082	5904	Reach_2771	1677	221	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-7.6	-8.5	-10.6
2-nitrophenol	201-857-5	88-75-5	88755	988	Reach_332	1678	139	70.8	6.4E+00	1.0E+04	8.1E+01	7.5		2.7E-08	1.1E-07	3.5E-07				22%	-8.8	-8.5	-9.6
2-ethyl-4-methylimidazole	230-786-2	7320-37-8	7320378	3615	Reach_2236	1679	240	51.3	2.9E-01	1.5E-02	5.8E+06	0	0	1.1E-06	1.1E-07	3.5E-07				16%	-8.6	-8.5	-10.4
triclocarban	202-924-1	101-20-2	101202	143	Reach_574	1680	316	182.0	4.8E-07	6.2E-01	7.9E+04	13.6		2.2E-09	1.1E-08	1.1E-08				24%	-8.0	-8.5	-9.4
tetrahydrofurfuryl alcohol	202-625-6	97-99-4	97994	1062	Reach_493	1681	102	-20.9	3.6E+01	3.4E+05	7.8E-01	15		1.6E-06	3.5E-07	1.1E-06				14%	-8.6	-8.5	-10.5
(S)-2-amino-3-(3,4-dimethoxyphenyl)-2-methylpropiononitrile	202-594-9	97-61-0	97610	1058	Reach_482	1682	116	15.2	5.7E+01	2.9E+04	9.5E+01									18%	-8.2	-8.5	-10.2
4-(methylthio)-3,5-xylenol	265-747-9	65405-84-7	65405847	3453	Reach_2873	1683	208	43.0	8.3E-01	2.5E+01	1.6E+05			3.5E-07	1.1E-07	3.5E-07				15%	-8.7	-8.5	-10.4
tert-butyl 3-(6-amino-3-methylpyridin-2-yl)benzoate	207-100-5	434-16-2	434162	2912	Reach_1273	1684	385	167.4	1.1E-07	7.4E-03	4.5E+08			1.1E-06	1.1E-07	3.5E-07				15%	-8.0	-8.5	-10.4
piperazine, compound with phosphoric acid	230-745-9	7300-34-7	7300347	3612	Reach_2235	1685	204	87.1	7.2E-02	6.2E+05	6.3E-01									18%	-8.2	-8.5	-10.2
3,3,5-trimethylcyclohexanol	204-122-7	116-02-9	116029	1642	Reach_949	1686	142	2.7	6.1E+00	9.3E+02	8.5E+02	16		1.1E-06	1.1E-07	3.5E-07				15%	-8.8	-8.5	-10.1
7-methoxy-4,4-dimethyl-1H-2-benzopyran-1,3(4H)-dione	603-200-1	127337-60-4	127337604	5648	Reach_4112	1687	276	0.0												15%	-8.7	-8.5	-10.4
(1R)-1-(3-methoxyphenyl)ethanamine	618-965-7	937203-35-5	937203355	4081	Reach_4504	1688	254	161.5	6.9E-05	5.1E+01	3.0E+00		6.95	1.1E-06	1.1E-07	1.1E-06				14%	-8.7	-8.5	-10.3
(1S)-1-(4-methoxyphenyl)ethanamine	298-842-9	93839-71-5	93839715	4089	Reach_3001	1689	262	134.1	2.3E-04	8.5E+02	2.2E+02		4.25	3.5E-06	3.5E-07	1.1E-06				14%	-8.7	-8.5	-10.3
606-907-3	222-746-8	3598-16-1	3598161	5858	Reach_1975	1690	174	0.0												14%	-8.7	-8.5	-10.3
benzyldimethylamine	203-149-1	103-83-3	103833	164	Reach_615	1691	135	-12.8	1.2E+02	1.7E+03	5.6E+01		5	1.7E-07	3.5E-08	1.1E-07				18%	-8.8	-8.5	-9.9
1-ethylpyrrolidin-2-one	220-250-6	2687-91-4	2687914	2489	Reach_1853	1692	113	30.0	1.4E+01	4.8E+04	2.4E+00		14.3	3.5E-06	3.5E-07	3.5E-06				14%	-8.7	-8.5	-10.4
diethyl [4-(prop-2-yn-1-yloxy)benzylidene]propanedioate	207-959-6	503-01-5	503015	3001	Reach_1301	1693	141	-38.6	1.5E+02	7.8E+03	1.1E+03			3.5E-07	3.5E-08	1.1E-07				15%	-8.7	-8.5	-10.4
4-methylthiosemicarbazide	229-563-2	6610-29-3	6610293	3462	Reach_2197	1694	105	29.5	3.8E+01	1.0E+06	6.2E-02	11.9	12.2	1.1E-06	3.5E-07	1.1E-06				14%	-7.4	-8.5	-10.5
4'-methoxyacetophenone	689-404-1	96240-10-7	96240107	4142	Reach_4651	1695	142	123.6	2.3E-03	8.2E+04	9.1E-02			1.1E-06	3.5E-07	1.1E-06				14%	-8.8	-8.5	-10.4
N'-[3-(dimethylamino)propyl]-N,N-dimethylpropane-1,3-diamir	229-761-9	6711-48-4	6711484	3485	Reach_2203	1696	187	36.6	4.7E+00	1.6E+05	1.6E+00		2.3	1.1E-06	1.1E-07	1.1E-06				14%	-8.5	-8.5	-10.5
tridecanedioic acid	208-011-4	505-52-2	505522	3008	Reach_1308	1697	244	150.4	2.1E-04	1.3E+02	4.7E+03	4.6		1.1E-06	1.1E-07	3.5E-07				14%	-8.0	-8.5	-10.5
dimethyl acetylsuccinate	202-550-9	96-99-1	96991	4160	Reach_475	1698	202	125.6	5.8E-04	5.0E+02	2.2E+02	3.17		1.1E-06	3.5E-08	1.1E-07				14%	-8.7	-8.5	-10.6
tert-butyl perbenzoate	210-382-2	614-45-9	614459	3334	Reach_1424	1699	194	34.0	3.1E+00	3.3E+02	7.8E+02			1.1E-06	1.1E-07	3.5E-07				15%	-8.8	-8.5	-10.1
2-tert-butylphenol	201-807-2	88-18-6	88186	983	Reach_318	1700	150	36.9	7.1E+00	1.3E+03	2.6E+03	10.8		2.2E-09	3.5E-07	1.1E-06				23%	-8.8	-8.5	-9.7
bis(2-ethylhexyl) azelate	203-091-7	103-24-2	103242	1361	Reach_604	1701	413	40.5	5.0E-04	1.6E-03	3.9E+09			1.1E-06	1.1E-07	3.5E-07				23%	-8.5	-8.5	-9.5
3,4,5-trimethoxytoluene	229-239-0	6443-69-2	6443692	3435	Reach_2187	1702	182	46.1	2.3E+00	1.1E+03	1.1E+02			1.1E-06	1.1E-07	3.5E-07				14%	-8.8	-8.5	-10.3

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
isopropyl myristate	203-751-4	110-27-0	110270	1516	Reach_810	1703	270	44.4	1.1E-01	6.2E-02	1.5E+07			1.1E-06	1.1E-07	3.5E-07				22%	-8.6	-8.5	-10.7
(1E)-1-(methoxyimino)-1-(2,5,5-trimethyl-1,3-dioxan-2-yl)acetc	619-753-7	73611-02-6	73611026	3625	Reach_4542	1704	142	50.6	6.8E-02	1.1E+07	2.9E+00			3.5E-06	3.5E-07	1.1E-06				15%	-8.7	-8.5	-10.4
2-chloroacetamide	201-174-2	79-07-2	79072	3765	Reach_227	1705	94	41.6	1.4E+00	9.2E+04	2.6E-01	13	16	3.5E-07	1.1E-07	3.5E-07				16%	-7.4	-8.5	-10.4
3,6,7-trimethyloct-6-en-1-yn-3-ol	201-368-7	81-64-1	81641	3808	Reach_276	1706	240	181.4	9.5E-08	1.1E+03	8.7E+03	10		3.5E-06	3.5E-07	1.1E-06				15%	-8.7	-8.5	-10.4
thymidine	200-070-4	50-89-5	50895	3021	Reach_10	1707	242	226.6	1.8E-11	5.2E+03	2.3E-01	9.71		3.5E-06	3.5E-07	1.1E-06				14%	-7.4	-8.5	-10.7
hexamethyldisiloxane	203-492-7	107-46-0	107460	1463	Reach_709	1708	162	-79.1	5.2E+03	1.5E+01	1.8E+05			3.5E-09	3.5E-09	3.5E-09				24%	-9.0	-8.5	-11.2
2,2'-p-phenylenedioxydiethanol	203-197-3	104-38-1	104381	1393	Reach_621	1709	198	102.9	8.8E-05	1.1E+05	4.1E+00	14.5		1.1E-06	1.1E-07	3.5E-07				14%	-7.5	-8.5	-10.6
629-935-8	629-935-8	32539-82-5	32539825	2654	Reach_4597	1710	240	100.0	5.1E-05	5.5E+00	1.0E+04	15.8		1.1E-06	1.1E-07	3.5E-07				16%	-8.3	-8.5	-10.4
bis(2-chloroethyl) ether	620-019-3	1124-64-7	1124647	5611	Reach_4556	1711	172	0.0												22%	-8.8	-8.5	-9.8
dihydrogen bis(acetato-O)difluoroborate(1-)	206-768-5	373-61-5	373615	5865	Reach_1260	1712	188	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.2	-8.5	-10.2
2,2'-azobis[2-methylbutyronitrile]	236-740-8	13472-08-7	13472087	1882	Reach_2338	1713	192	64.1	1.2E-01	1.4E+02	7.2E+03			3.5E-07	3.5E-08	1.1E-07				17%	-8.8	-8.5	-10.2
dimethyl sulphide	200-846-2	75-18-3	75183	853	Reach_133	1714	62	-107.7	6.4E+04	1.5E+04	8.3E+00			2.2E-09	3.5E-08	3.5E-07				24%	-8.9	-8.5	-10.7
N,N'-(2-chloro-5-methyl-1,4-phenylene)bis[3-oxobutyramide]	201-100-9	78-27-3	78273	893	Reach_197	1715	124	21.6	3.6E+01	2.6E+03	6.5E+01	13.6	0	7.4E-09	3.5E-07	1.1E-06				16%	-7.5	-8.5	-10.4
bis(pentane-2,4-dionato-O,O')bis(propan-2-olato)titanium	230-191-8	6969-71-7	6969717	3548	Reach_2216	1716	135	122.0	2.7E-03	4.1E+04	2.8E+00									18%	-8.2	-8.5	-10.2
octanoyl chloride	203-891-6	111-64-8	111648	1551	Reach_862	1717	163	-6.7	8.5E+01	3.6E+01	3.0E+02			1.1E-06	1.1E-07	3.5E-07				18%	-8.8	-8.5	-10.9
2,5-dianilinoterephthalic acid	233-302-8	10109-95-2	10109952	1314	Reach_2282	1718	348	242.1	4.0E-10	1.2E+02	3.0E+04	3.7	14.5	1.1E-06	3.5E-07	1.1E-06				14%	-7.9	-8.5	-10.4
6-[(p-tosyl)amino]hexanoic acid, compound with 2,2',2''-nitrilo	301-097-5	93981-14-7	93981147	6086	Reach_3005	1719	435	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.2	-8.5	-10.2
diethyl maleate	600-786-0	106904-09-0	106904090	1448	Reach_4075	1720	249	157.2	7.3E-05	3.9E+02	1.9E+01			1.1E-06	1.1E-07	3.5E-07				15%	-8.8	-8.5	-10.1
tetramethyl 2,2'-[1,4-phenylenebis[imino(1-acetyl-2-oxoethane	271-176-6	68516-73-4	68516734	3518	Reach_2907	1721	717	349.8	6.7E-21	1.5E-02	2.2E+03	8.26	13.5	1.1E-06	1.1E-07	3.5E-07				14%	-7.9	-8.5	-10.5
bis(2,4,4-trimethylpentyl)phosphinic acid	619-785-1	249561-98-6	249561986	5794	Reach_4545	1722	307	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				19%	-8.3	-8.5	-10.1
1-cyanoallyl acetate	201-855-4	88-74-4	88744	987	Reach_331	1723	138	71.6	2.2E-01	1.2E+03	1.0E+02			2.2E-09	1.1E-07	3.5E-07				14%	-8.8	-8.5	-10.3
608-497-1	611-000-0	5344-48-9	5344489	5922	Reach_4345	1724	285	0.0												16%	-7.7	-8.5	-10.3
606-097-1	606-097-1	186817-80-1	186817801	2203	Reach_4193	1725	202	28.4	1.2E-01	8.0E+02	4.9E+02	12.6		3.5E-06	3.5E-07	1.1E-06				14%	-8.8	-8.5	-10.4
2-phenoxyethyl isobutyrate	203-127-1	103-60-6	103606	1374	Reach_609	1726	208	37.7	7.0E-01	3.9E+02	1.0E+03			3.5E-07	1.1E-07	3.5E-07				16%	-8.8	-8.5	-10.2
diammonium 2,2'-dithiodiacetate	269-323-4	68223-93-8	68223938	5995	Reach_2901	1727	216	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.2	-8.5	-10.2
fluorobenzene	207-321-7	462-06-6	462066	643	Reach_1285	1728	96	-73.0	9.6E+03	9.0E+02	1.5E+02			2.2E-09	1.1E-07	3.5E-07				24%	-8.9	-8.5	-11.0
2,2'-methylenediphenyl diisocyanate	219-799-4	2536-05-2	2536052	1249	Reach_1833	1729	250	98.7	6.3E-03	3.5E+01	1.7E+05			1.1E-06	1.1E-07	3.5E-07				18%	-8.6	-8.5	-10.3
N-(3-{[(dimethyl(3-[(2-methylacryloyl)amino]propyl)ammonio)	700-055-7	630113-05-2	630113052	5959	Reach_4743	1730	537	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.2	-8.5	-10.2
3-hydroxy-2'-methyl-2-naphthanilide	205-205-0	135-61-5	135615	1893	Reach_1132	1731	277	210.7	6.6E-09	4.3E-01	2.9E+04	10.2		1.1E-06	3.5E-08	1.1E-07				16%	-7.8	-8.5	-10.3
N,N,N',N',N'',N''-hexamethyl-1,3,5-triazine-1,3,5(2H,4H,6H)-trip	240-004-1	15875-13-5	15875135	2064	Reach_2403	1732	343	162.2	5.9E-05	5.2E+03	2.6E-02		4.08	3.5E-06	1.1E-07	3.5E-07				14%	-7.5	-8.5	-10.8
cis-2,6-dimethylmorpholine	202-282-2	93-84-5	93845	4090	Reach_408	1733	179	148.3	5.0E-04	4.2E+03	1.0E+01			1.1E-06	3.5E-08	1.1E-07				14%	-8.8	-8.5	-10.3
benzophenone-3,3':4,4'-tetracarboxylic dianhydride	214-012-0	1072-63-5	1072635	1457	Reach_1642	1734	94	12.7	2.5E+01	4.6E+04	9.1E+00			3.5E-07	3.5E-08	1.1E-07				15%	-7.8	-8.5	-10.4
dimethyl maleate	210-848-5	624-48-6	624486	3369	Reach_1452	1735	144	-95.9	1.1E+01	1.8E+04	1.6E+01			3.5E-06	3.5E-07	1.1E-06				14%	-8.8	-8.5	-10.5
2-ethylhexyl stearate	244-754-0	22047-49-0	22047490	2316	Reach_2515	1736	397	135.2	2.3E-05	3.3E-06	3.9E+11			1.1E-06	1.1E-07	3.5E-07				24%	-8.8	-8.5	-9.2
3-oxopregn-4-ene-21,17α-carbolactone	213-552-4	976-70-5	976705	4169	Reach_1622	1737	342	187.6	1.0E-06	2.6E+01	1.7E+04			1.1E-06	1.1E-07	3.5E-07				16%	-7.8	-8.5	-10.3
3-hydroxy-2,2-dimethylpropyl 3-hydroxy-2,2-dimethylpropiona	212-876-3	875-74-1	875741	3936	Reach_1583	1738	151	238.7	3.7E-06	4.4E+04	1.7E-02	1.8		3.5E-06	3.5E-07	1.1E-06				14%	-7.7	-8.5	-10.5
α,α,α-trifluoro-m-cresol	202-645-5	98-17-9	98179	1069	Reach_502	1739	162	13.5	8.1E+01	6.0E+03	3.0E+02	8.8		3.5E-09	1.1E-06	3.5E-06				23%	-8.8	-8.5	-9.8
601-332-4	603-436-5	13076-17-0	13076170	1843	Reach_4121	1740	144	26.1	2.1E-02	1.5E+07	4.5E+01			3.5E-06	3.5E-07	1.1E-06				16%	-7.8	-8.5	-10.3
1,1,1,3,3-pentachlorobutane	244-691-9	21981-33-9	21981339	2314	Reach_2512	1741	230	-1.1	2.9E+02	3.6E+01	5.8E+04			1.1E-07	1.1E-08	3.5E-08				23%	-8.9	-8.5	-11.1
hex-3-yne-2,5-diol	206-687-5	367-25-9	367259	2774	Reach_1253	1742	129	4.1	2.1E+02	2.5E+03	3.0E+01	0		1.1E-06	1.1E-07	3.5E-07				14%	-7.5	-8.5	-10.6
ethyl chloroformate	208-778-5	541-41-3	541413	3129	Reach_1340	1743	109	-69.2	6.2E+03	1.4E+04	4.3E+00			3.5E-06	3.5E-07	1.1E-06				14%	-8.8	-8.5	-10.6
1,2-diphenoxyethane	204-847-9	127-52-6	127526	1186	Reach_1099	1744	214	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				17%	-8.8	-8.6	-10.2
tridecane	211-093-4	629-50-5	629505	3389	Reach_1467	1745	184	-9.6	1.2E+01	1.2E-02	5.4E+06			3.5E-07	3.5E-08	1.1E-07				23%	-8.8	-8.6	-11.2
panthenol , DL-form	240-540-6	16485-10-2	16485102	2094	Reach_2422	1746	205	161.4	2.0E-06	1.3E+05	1.2E-02	13.2	15.5	1.1E-06	3.5E-07	1.1E-06				14%	-7.3	-8.6	-10.5
amantadine	229-713-7	6674-22-2	6674222	3481	Reach_2201	1747	152	40.6	7.4E+00	5.2E+03	5.0E+02		1.6	3.5E-07	1.1E-07	3.5E-07				18%	-8.8	-8.6	-10.1
diallyl carbonate	219-340-8	2420-17-9	2420179	2377	Reach_1802	1748	192	197.9	5.1E-08	5.6E+03	1.0E+00			1.1E-05	1.1E-06	3.5E-06				15%	-8.8	-8.6	-10.0
chlorocresol	220-672-0	2857-97-8	2857978	2538	Reach_1877	1749	153	-75.3	1.3E+04	7.4E+02	3.7E+02	0		3.5E-09	3.5E-09	3.5E-09				23%	-8.8	-8.6	-9.6
dibutyl phosphonate	217-316-1	1809-19-4	1809194	2164	Reach_1722	1750	194	17.4	3.2E+00	6.8E+04	6.5E+01			1.1E-06	1.1E-07	3.5E-07				14%	-8.7	-8.6	-10.5
Ammonium 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propan	700-242-3	62037-80-3	62037803	5953	Reach_4817	1751	347	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.2	-8.6	-10.2
L-valine	200-773-6	72-18-4	72184	3599	Reach_105	1752	117	252.1	1.2E-06	4.0E+04	8.3E-03	2.3	4.2	3.5E-06	3.5E-07	1.1E-06				14%	-7.2	-8.6	-10.6
2,4-dichloro-5-isopropoxyaniline	255-258-9	41200-96-8	41200968	2871	Reach_2739	1753	220	85.6	6.4E-02	4.6E+01	2.2E+03		12.5	1.1E-06	1.1E-07	3.5E-07				14%	-8.0	-8.6	-10.6
4-cyanophenyl acetate	235-893-8	13031-41-9	13031419	1835	Reach_2318	1754	161	54.0	6.9E-01	1.2E+03	1.4E+01			1.1E-06	3.5E-07	1.1E-06				14%	-8.8	-8.6	-10.4
oleonitrile	204-016-0	112-91-4	112914	1610	Reach_929	1755	263	88.4	9.5E-03	9.3E-04	3.2E+07			1.1E-06	1.1E-07	3.5E-07				23%	-8.6	-8.6	-10.9
tert-butyl (1R,3S,4S)-3-(5-bromo-1H-benzimidazol-2-yl)-2-azabi	700-743-7	161798-03-4	161798034	2082	Reach_4983	1756	347	194.4	5.8E-07	5.1E-01	6.8E+04		12.2	1.1E-06	1.1E-07	3.5E-07				16%	-7.8	-8.6	-10.3
valeraldehyde	203-784-4	110-62-3	110623	280	Reach_821	1757	86	-67.5	4.4E+03	2.5E+04	2.0E+01			4.1E-06	1.1E-06	3.5E-06				14%	-8.8	-8.6	-10.3
613-982-6	249-020-3	28443-50-7	28443507	2530	Reach_2617	1758	144	69.8	1.9E-01	4.4E+03	1.7E+01			1.1E-06	1.1E-07	3.5E-07				15%	-8.8	-8.6	-10.4
diethyl peroxydicarbonate	238-707-3	14666-78-5	14666785	1992	Reach_2367	1759	178	-4.9	1.2E+00	5.3E+03	1.7E+01			1.1E-06	1.1E-07	3.5E-07				14%	-8.8	-8.6	-10.5
trimethoxyphenylsilane	221-066-9	2996-92-1	2996921	2582	Reach_1894	1760	198	20.2	9.7E+00	7.9E+02	3.5E+00			3.5E-07	1.1E-07	3.5E-07				16%	-8.8	-8.6	-10.0
2-phenoxyethyl acrylate	256-360-6	48145-04-6	48145046	2972	Reach_2760	1761	192	36.5	1.1E+00	5.8E+02	2.9E+02			1.1E-06	1.1E-07	3.5E-07				15%	-8.8	-8.6	-10.4
N-(1,1,3,3-tetramethylbutyl)acrylamide	224-169-7	4223-03-4	4223034	1266	Reach_2021	1762	183	83.7	8.8E-02	2.2E+02	7.4E+02	15.1	14.4	1.1E-06	3.5E-07	1.1E-06				15%	-8.8	-8.6	-10.4
isobutyl methacrylate	202-613-0	97-86-9	97869	4174	Reach_489	1763	142	-54.0	4.2E+02	1.4E+03	4.7E+02			3.5E-06	3.5E-07	1.1E-06				15%	-8.8	-8.6	-10.5
(1S,7S,8S,8aR)-8-(2-[(2R,4R)-4-hydroxy-6-oxotetrahydro-2H-py	691-746-1	220380-44-9	220380449	1241	Reach_4671	1764	1618	0.0												16%	-7.8	-8.6	-10.3
N,N-dimethyldecan-1-amide	238-405-1	14433-76-2	14433762	471	Reach_2366	1765	199	60.8	2.1E-01	1.3E-01	2.8E+03		14	4.0E-07	3.5E-08	1.1E-07				20%	-8.9	-8.6	-10.7
609-118-2	600-451-9	103577-40-8	103577408	1371	Reach_4064	1766	353	215.8	2.3E-08	7.8E-01	2.7E+04		8.54	3.5E-07	1.1E-07	3.5E-07				16%	-8.6	-8.6	-10.4
5-hydroxyisophthalic acid	606-793-5	21535-43-3	21535433	2297	Reach_4218	1767	260	170.2	5.5E-06	3.6E+00	1.4E+03	12.7		1.1E-06	1.1E-07	3.5E-07				14%	-7.6	-8.6	-10.5
triacetoxyethylsilane	241-677-4	17689-77-9	17689779	2148	Reach_2441	1768	234	-33.7	1.0E+01	3.7E+03	5.5E+00			3.5E-06	3.5E-07	1.1E-06				14%	-8.8	-8.6	-10.4
triethoxy(phenyl)silane	212-305-8	780-69-8	780698	891	Reach_1546	1769	240	52.1	3.7E-01	6.4E+01	1.0E+02			2.6E-07	3.5E-08	1.1E-07				17%	-8.8	-8.6	-10.0
glutamic acid	200-293-7	56-86-0	56860	3214	Reach_32	1770	147	228.4	1.5E-04	3.3E+05	1.5E-04	2.08	3.98	3.5E-06	3.5E-07	1.1E-06				14%	-7.3	-8.6	-10.7
tetrahydro-4-methylphthalic anhydride	251-823-9	34090-76-1	34090761	2690	Reach_2670	1771	166	25.3	2.6E+00	5.3E+03	4.6E+03			3.5E-06	3.5E-07	1.1E-06				15%	-8.8	-8.6	-10.4
pseudoephedrine	202-018-6	90-82-4	90824	4008	Reach_368	1772	165	40.5	1.4E+00	1.4E+04	4.8E+00	13.5	4.6	1.1E-06	1.1E-07	3.5E-07				14%	-8.7	-8.6	-10.6
triethyl orthoformate	204-550-4	122-51-0	122510	1750	Reach_1029	1773	148	-38.3	9.3E+02	3.3E+04	2.8E+01			3.5E-07	1.1E-07	3.5E-07				16%	-8.8	-8.6	-9.9
(1S)-1-(3-methoxyphenyl)ethanamine	619-058-9	94695-48-4	94695484	4107	Reach_4509	1774	213	23.2	1.2E+02	1.9E+02	1.7E+02			1.1E-06	3.5E-07	1.1E-06				14%	-8.8	-8.6	-10.3
DL-malic acid	210-514-9	617-48-1	617481	3352	Reach_1435	1775	134	112.7	3.9E-04	3.4E+05	2.1E-02	3.63		3.5E-06	3.5E-07	1.1E-06				14%	-7.3	-8.6	-10.6
diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide	278-355-8	75980-60-8	75980608	3692	Reach_2946	1776	348	89.7	3.9E-06	2.7E-01	7.4E+03			3.5E-07	3.5E-08	1.1E-07				17%	-8.6	-8.6	-10.3
2-[(4-chloro-2-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxobu	236-852-7	13515-40-7	13515407	1887	Reach_2340	1777	391	239.2	6.2E-10	1.9E+00	3.5E+03	8.58	14.1	3.5E-07	1.1E-07	3.5E-07				17%	-7.9	-8.6	-10.3

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
dimethyl 5-methylpyridine-2,3-dicarboxylate	214-625-3	1170-02-1	1170021	1654	Reach_1665	1778	360	323.7	1.2E-14	5.4E-01	3.3E-03		4.76	1.1E-06	1.1E-07	3.5E-07				14%	-8.8	-8.6	-10.4
N,N'-dithiodi-o-phenylenedibenzamide	205-201-9	135-57-9	135579	1891	Reach_1131	1779	457	315.9	3.2E-15	1.3E-02	3.9E+04	14.4	12.9	1.1E-06	3.5E-07	1.1E-06				14%	-7.9	-8.6	-10.5
6,6'-di-tert-butyl-4,4'-thiodi-m-cresol	202-525-2	96-69-5	96695	4152	Reach_469	1780	359	196.9	2.9E-08	1.3E-02	1.7E+08	10.5		1.1E-06	1.1E-07	3.5E-07				23%	-8.1	-8.6	-9.4
ethyl chloroacetate	203-294-0	105-39-5	105395	173	Reach_639	1781	123	-48.6	7.0E+02	2.1E+04	1.3E+01			2.4E-07	3.5E-07	1.1E-06				17%	-8.9	-8.6	-9.9
2-(3,6-dihydroxy-2,4,5,7-tetrabromoxanthen-9-yl)-benzoic acid	604-351-6	143390-89-0	143390890	470	Pest_74	1782	313	137.4	1.7E-04	4.2E+00	7.6E+05			7.1E-07	1.1E-07	3.5E-07				20%	-8.1	-8.6	-10.3
N,N,N-trimethylanilinium chloride	260-126-9	56358-17-9	56358179	3192	Reach_2814	1783	255	114.1	1.0E-03	3.6E-02	1.4E+06									18%	-8.3	-8.6	-10.2
pin-2(10)-ene	204-872-5	127-91-3	127913	412	Reach_1102	1784	136	-15.3	3.3E+02	1.8E+01	2.2E+04			1.1E-08	3.5E-08	3.5E-08				24%	-8.9	-8.6	-11.2
N,N-dimethyldecylamine N-oxide	220-020-5	2605-79-0	2605790	2452	Reach_1844	1785	201	152.6	4.6E-05	1.0E+01	4.9E+03		9.2	3.5E-07	3.5E-08	1.1E-07				16%	-8.2	-8.6	-10.5
phenyl isocyanate	228-528-9	6289-46-9	6289469	3381	Reach_2161	1786	228	35.9	7.4E-02	5.1E+04	1.0E-02			3.5E-06	3.5E-07	1.1E-06				15%	-8.9	-8.6	-10.2
1-(1,3-benzodioxol-5-yl)propan-1-one	248-937-6	28281-49-4	28281494	2526	Reach_2616	1787	178	68.7	2.9E-01	1.9E+03	1.7E+02			1.1E-06	1.1E-07	3.5E-07				15%	-8.8	-8.6	-10.5
2,6-di-tert-butylphenol	204-884-0	128-39-2	128392	1820	Reach_1109	1788	206	77.0	9.4E-01	1.3E+01	3.0E+04	11.3		3.5E-06	3.5E-07	1.1E-06				16%	-8.9	-8.6	-10.3
3-(isodecyloxy)propiononitrile	613-099-6	62889-66-1	62889661	3379	Reach_4380	1789	316	137.2	8.0E-07	5.4E-02	1.7E+05			1.1E-06	1.1E-07	3.5E-07				17%	-8.9	-8.6	-9.9
604-018-5	604-018-5	137433-01-3	137433013	5682	Reach_4137	1790	584	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.3	-8.6	-10.3
[4-[α-[4-(dimethylamino)phenyl]benzylidene]cyclohexa-2,5-die	255-288-2	41272-40-6	41272406	5879	Reach_2742	1791	389	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.3	-8.6	-10.3
4'-aminoazobenzene-4-sulphonic acid	203-187-9	104-23-4	104234	1388	Reach_620	1792	277	196.8	1.9E-09	5.2E+02	1.1E+00	0.4	11.1	1.1E-06	3.5E-07	1.1E-06				14%	-7.6	-8.6	-10.6
3,3-Dimethoxy-8,8,9,9-tetramethyl-2-oxa-7-thia-3,8-disiladecar	700-413-2	6331-96-0	6331960	3399	Reach_4891	1793	242	156.7	1.1E-06	3.5E+01	1.6E-01			1.1E-07	1.1E-08	3.5E-08				15%	-8.9	-8.6	-10.5
diphenyl methylphosphonate	231-388-1	7526-26-3	7526263	3659	Reach_2257	1794	248	84.8	9.9E-03	2.4E+01	8.9E+02			3.5E-07	1.1E-07	3.5E-07				16%	-8.9	-8.6	-10.4
ethyl 3-ethoxypropionate	212-112-9	763-69-9	763699	3710	Reach_1537	1795	146	-26.9	2.0E+02	1.8E+04	1.2E+01			3.5E-06	3.5E-07	1.1E-06				14%	-8.8	-8.6	-10.3
cyclododecanol	217-031-2	1724-39-6	1724396	2126	Reach_1713	1796	184	25.5	1.7E-02	1.0E+01	3.8E+04	16		1.1E-06	1.1E-07	3.5E-07				17%	-8.8	-8.6	-10.4
xylitol	201-788-0	87-99-0	87990	3944	Reach_315	1797	152	102.7	2.6E-01	1.0E+06	2.8E-03	13.4		3.5E-06	1.1E-06	3.5E-06				14%	-7.7	-8.6	-10.7
2-aminobutan-1-ol	202-488-2	96-20-8	96208	4141	Reach_454	1798	89	-14.7	3.6E+01	8.3E+05	2.0E-01	15	4.5	3.5E-06	1.1E-06	3.5E-06				14%	-8.5	-8.6	-10.6
3-amino-2-hydroxy-5-nitrobenzenesulphonic acid	202-523-1	96-67-3	96673	4151	Reach_468	1799	234	191.0	1.1E-08	2.8E+03	6.8E-03	-1.75	12.4	3.5E-06	1.1E-07	3.5E-07				14%	-7.3	-8.6	-10.8
2-chloro-6-nitrotoluene	700-290-5	63968-64-9	63968649	3421	Reach_4844	1800	282	132.8	2.9E-04	1.5E+02	7.1E+02			3.5E-06	3.5E-07	1.1E-06				23%	-8.9	-8.6	-10.0
diisodecyl maleate	258-806-5	53817-61-1	53817611	3111	Reach_2794	1801	397	26.1	7.7E-04	9.7E-04	8.1E+09			1.1E-06	1.1E-07	3.5E-07				23%	-8.6	-8.6	-9.6
isobutyl (S)-2-chloropropionate	280-349-5	83261-15-8	83261158	3844	Reach_2965	1802	165	-38.8	2.2E+02	1.2E+03	2.8E+02			3.5E-06	3.5E-07	1.1E-06				14%	-8.9	-8.6	-10.5
ditetradecyl fumarate	233-739-4	10341-03-4	10341034	1364	Reach_2289	1803	509	136.7	1.3E-07	6.5E-08	9.5E+13			1.1E-06	1.1E-07	3.5E-07				24%	-8.9	-8.6	-8.5
3-amino-4-hydroxy-5-nitrobenzenesulphonic acid	251-868-4	34184-82-2	34184822	2693	Reach_2672	1804	328	179.1	9.0E-08	1.6E+02	1.0E+03	13.9		3.5E-07	3.5E-08	1.1E-07				14%	-7.3	-8.6	-10.8
2,3-epoxypropyl methacrylate	203-441-9	106-91-2	106912	1449	Reach_681	1805	142	-23.3	8.3E+01	2.6E+04	6.5E+00			3.5E-06	3.5E-07	1.1E-06				14%	-8.8	-8.6	-10.4
608-245-0	608-245-0	28770-01-6	28770016	2544	Reach_4267	1806	159	44.9	4.5E-01	1.9E+05	1.1E+00	14.9	5.8	1.1E-06	3.5E-07	1.1E-06				14%	-7.9	-8.6	-10.6
cyclohexanone oxime	209-378-3	574-93-6	574936	3230	Reach_1378	1807	515	349.8	5.0E-19	4.9E-06	4.9E+07	0		1.1E-07	3.5E-09	1.1E-08				17%	-8.6	-8.6	-10.4
3,3'-Diisopropyl-5,5',6,6'-tetramethylbiphenyl-2,2'-diol	202-772-6	99-61-6	99616	1090	Reach_533	1808	151	69.5	6.0E-01	1.1E+03	3.4E+01			6.6E-08	3.5E-08	1.1E-07				23%	-8.2	-8.6	-9.2
naphthalene-1,8-dicarboximide	610-979-1	53207-58-2	53207582	3091	Reach_4343	1809	194	50.7	3.4E-01	4.2E+01	1.5E+03	0	0	3.5E-07	1.1E-07	3.5E-07				16%	-7.6	-8.6	-10.6
2,2'-(octadec-9-enylimino)bisethanol	246-807-3	25307-17-9	25307179	2429	Reach_2565	1810	356	174.2	4.3E-09	8.5E-04	4.3E+06	14.7	4.7	1.1E-06	3.5E-07	1.1E-06				21%	-8.1	-8.6	-9.9
2,3-dihydroxypropyl laurate	205-526-6	142-18-7	142187	1949	Reach_1173	1811	274	121.1	5.1E-06	1.1E+01	4.7E+03	13.5		1.1E-06	3.5E-07	1.1E-06				15%	-8.0	-8.6	-10.5
610-950-3	611-813-0	5926-26-1	5926261	3271	Reach_4365	1812	171	-27.1	3.4E+02		3.8E-01			1.1E-06	3.5E-07	1.1E-06				19%	-8.9	-8.6	-10.0
2-[(4-chloro-2-nitrophenyl)azo]-N-(2-chlorophenyl)-3-oxobutyr	229-355-1	6486-23-3	6486233	3446	Reach_2191	1813	395	236.9	8.9E-10	6.1E-02	1.3E+04	8.58		3.5E-07	1.1E-08	3.5E-08				17%	-7.8	-8.6	-10.4
dioctadecyl disulphide	219-702-5	2500-88-1	2500881	2411	Reach_1824	1814	571	241.3	1.0E-10	4.2E-12	3.7E+18			1.1E-06	1.1E-07	3.5E-07				24%	-8.9	-8.6	-6.4
N,N'-ethylenebis(3,4,5,6-tetrabromophthalimide)	251-118-6	32588-76-4	32588764	2656	Reach_2663	1815	952	349.8	1.8E-21	1.5E-08	6.3E+09			1.1E-06	1.1E-07	3.5E-07				23%	-8.6	-8.6	-9.2
2-nitro-p-toluidine	201-924-9	89-62-3	89623	991	Reach_347	1816	152	84.5	6.0E-02	3.5E+02	3.7E+02		14	2.9E-09	3.5E-08	1.1E-07				23%	-8.9	-8.6	-9.6
propyl chloroformate	210-438-6	615-60-1	615601	3339	Reach_1428	1817	141	-9.4	6.5E+01	2.5E+01	5.4E+03			3.5E-07	3.5E-08	1.1E-07				14%	-8.9	-8.6	-10.7
trichloro(vinyl)silane	200-917-8	75-94-5	75945	3690	Reach_167	1818	161	-65.5	7.2E+03		2.3E+02			1.1E-06	1.1E-07	3.5E-07				19%	-8.9	-8.6	-11.3
Octan-2-yl cyanoacetate	298-791-2	93839-21-5	93839215	4088	Reach_3000	1819	285	233.9	1.4E-09	4.4E+02	1.8E+01			3.5E-06	1.1E-07	3.5E-07				15%	-8.9	-8.6	-10.4
guanidinium chloride	203-533-9	107-93-7	107937	225	Reach_720	1820	86	2.4	3.3E+01	1.2E+05	7.1E+00		0	4.2E-06	3.5E-07	1.1E-06				14%	-8.8	-8.6	-10.5
nitromethane	200-876-6	75-52-5	75525	860	Reach_148	1821	61	-51.7	4.8E+03	7.2E+04	9.1E-01	10.1		2.2E-09	1.1E-07	3.5E-07				23%	-8.9	-8.6	-9.9
7,8-didehydrocholesterol	223-028-7	3698-89-3	3698893	2787	Reach_1983	1822	216	22.2	9.4E-01	9.5E-03	2.1E+06			3.5E-07	3.5E-08	1.1E-07				23%	-8.3	-8.6	-9.3
2-ethylhexyl diphenyl phosphate	214-987-2	1241-94-7	1241947	403	Reach_1675	1823	362	86.7	4.5E-03	9.0E-02	2.0E+06			1.3E-08	1.1E-07	3.5E-07				23%	-8.8	-8.6	-9.9
bis(2,3-epoxypropyl) terephthalate	230-565-0	7195-44-0	7195440	3595	Reach_2230	1824	278	65.2	8.1E-03	2.3E+03	5.5E+00			1.1E-06	1.1E-07	3.5E-07				14%	-8.0	-8.6	-10.7
5-vinylnorborn-2-ene	605-460-1	167004-78-6	167004786	2110	Reach_4176	1825	261	-44.7	1.0E-01	2.4E+03	7.1E-01			3.5E-06	3.5E-07	1.1E-06				18%	-8.9	-8.6	-11.1
diallyl phthalate	205-016-3	131-17-9	131179	418	Reach_1120	1826	246	15.8	1.5E-01	9.3E+01	2.3E+03			8.2E-07	1.1E-07	3.5E-07				15%	-8.9	-8.6	-10.4
2'-chloroacetoacetanilide	202-269-1	93-70-9	93709	4080	Reach_407	1827	212	134.5	9.4E-04	3.9E+03	1.2E+01	10.7		1.1E-06	1.1E-07	3.5E-07				14%	-7.7	-8.6	-10.7
3-3-diphenylpropylamine	255-670-9	42125-46-2	42125462	2889	Reach_2749	1828	219	22.9	5.7E+00	6.6E-01	1.5E+04			1.1E-06	1.1E-07	3.5E-07				15%	-8.9	-8.6	-10.4
dibutylamine	203-921-8	111-92-2	111922	317	Reach_882	1829	129	-29.9	3.4E+02	2.0E+03	5.9E+02		3	5.0E-07	1.1E-07	3.5E-07				16%	-8.9	-8.6	-10.2
2,2,2-trifluoroethanol	200-913-6	75-89-8	75898	866	Reach_165	1830	100	-91.0	1.0E+04	6.0E+05	1.9E+00	12.3		7.2E-07	1.1E-06	3.5E-06				15%	-8.9	-8.6	-10.0
pentamethylenediamine	207-329-0	462-94-2	462942	2950	Reach_1286	1831	102	12.9	1.3E+02	1.0E+06	7.1E-01		3.28	1.1E-06	3.5E-07	1.1E-06				14%	-8.8	-8.6	-10.6
bis(4-fluorophenyl) ketone	206-466-3	345-92-6	345926	2710	Reach_1240	1832	218	74.7	6.6E-02	1.5E+01	3.5E+03			1.1E-06	3.5E-08	1.1E-07				15%	-8.9	-8.6	-10.3
decanenitrile	217-830-6	1975-78-6	1975786	2239	Reach_1741	1833	153	11.4	5.3E+00	1.1E+02	6.0E+03			3.5E-07	3.5E-08	1.1E-07				17%	-8.9	-8.6	-9.9
(R)-p-mentha-1,8-diene	227-813-5	5989-27-5	5989275	743	Reach_2147	1834	136	-40.8	1.9E+02	7.7E+00	6.8E+04			5.7E-07	1.1E-07	3.5E-07				22%	-8.9	-8.6	-11.4
p-(2-methoxyethyl)phenol	260-354-9	56718-71-9	56718719	3211	Reach_2821	1835	152	47.1	1.0E+00	1.8E+03	6.2E+01	10		3.5E-06	3.5E-07	1.1E-06				14%	-8.9	-8.6	-10.6
4-diazo-3,4-dihydro-7-nitro-3-oxonaphthalene-1-sulphonic acid	205-583-7	143-08-8	143088	469	Reach_1189	1836	144	-3.2	4.4E+00	1.2E+02	2.0E+03	15.9		3.8E-06	3.5E-07	1.1E-06				14%	-7.4	-8.6	-10.8
nonan-4-olide	203-219-1	104-61-0	104610	1395	Reach_624	1837	156	9.8	1.6E+00	6.6E+02	1.2E+02			1.1E-06	1.1E-07	3.5E-07				15%	-8.9	-8.6	-10.4
p-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	225-716-2	5026-74-4	5026744	3000	Reach_2071	1838	277	127.5	7.6E-04	1.6E+03	7.4E+00		10.1	1.1E-06	1.1E-07	3.5E-07				14%	-7.7	-8.6	-10.7
2,2'-oxydi(ethylamine)	220-395-5	2752-17-2	2752172	2511	Reach_1863	1839	104	18.6	1.9E+02	3.7E+06	1.3E-02		4.28	1.1E-06	3.5E-07	1.1E-06				14%	-8.6	-8.6	-10.7
dibromomethane	200-824-2	74-95-3	74953	842	Reach_118	1840	174	-51.6	6.5E+03	1.1E+04	3.3E+01			2.0E-08	3.5E-08	1.1E-07				23%	-9.0	-8.6	-10.7
Ethyl N-pyridin-2-yl-beta-alaninate	201-756-6	87-60-5	87605	3937	Reach_312	1841	142	41.8	4.7E+00	5.1E+02	1.9E+02		10.5	1.1E-06	3.5E-07	1.1E-06				14%	-8.5	-8.7	-10.6
3-acetoxymethylen-7-amino-8-oxo-5-thia-1-azabicyclo[4.2.0]oc	213-485-0	957-68-6	957686	4133	Reach_1617	1842	272	305.3	5.1E-09	1.1E+04	4.7E-02	1.97	7.13	3.5E-06	3.5E-07	1.1E-06				14%	-7.3	-8.7	-10.7
N,N'-bis(1,3-dimethylbutylidene)-2,2'-iminobis(ethylamine)	234-205-3	10595-60-5	10595605	1423	Reach_2301	1843	267	1.1	8.3E-02	1.9E+01	4.3E+07		3.4	3.5E-06	3.5E-07	1.1E-06				21%	-8.4	-8.7	-9.9
607-449-7	607-449-7	24863-70-5	24863705	2405	Reach_4241	1844	224	85.7	2.8E-02	1.3E+02	2.0E+03			3.5E-07	1.1E-07	3.5E-07				17%	-8.9	-8.7	-10.4
diethyl malonate	203-305-9	105-53-3	105533	177	Reach_641	1845	160	-83.3	4.8E+01	4.1E+04	7.9E+00	13		1.0E-06	3.5E-07	1.1E-06				14%	-8.9	-8.7	-10.5
4-chloro-N-cyclopentylbenzylamine	700-544-5	641571-10-0	641571100	3427	Reach_4930	1846	530	331.0	2.7E-16	3.5E-05	1.0E+05		8.09	1.1E-06	1.1E-07	3.5E-07				19%	-8.9	-8.7	-10.2
2-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbon	250-830-4	31837-42-0	31837420	2639	Reach_2658	1847	381	288.0	2.9E-13	1.9E+02	5.6E+01	3.99	11.8	1.1E-06	1.1E-07	3.5E-07				14%	-7.8	-8.7	-10.7
dibenzylamine	203-117-7	103-49-1	103491	1368	Reach_607	1848	197	74.4	1.3E-01	1.2E+01	1.7E+03		5.6	1.1E-06	1.1E-07	3.5E-07				15%	-8.9	-8.7	-10.2
ethylene distearate	264-261-4	63469-23-8	63469238	3403	Reach_2859	1849	218	83.8	9.5E-04	1.9E+05	3.3E-01			3.5E-06	1.1E-07	1.1E-06				24%	-8.9	-8.7	-7.5
4'-methylacetophenone	204-514-8	122-00-9	122009	1740	Reach_1023	1850	134	7.9	1.1E+01	5.8E+02	1.7E+02			1.1E-06	1.1E-07	3.5E-07				15%	-8.9	-8.7	-10.1
heptane	205-563-8	142-82-5	142825	463	Reach_1180	1851	100	-81.0	6.1E+03	2.4E+01	6.0E+03			1.6E-06	3.5E-08	1.1E-07				20%	-9.0	-8.7	-11.7
3-bromopropene	202-728-6	99-08-1	99081	1082	Reach_526	1852	137	38.2	9.4E+00	2.8E+02	2.3E+02			3.9E-09	3.5E-08	1.1E-07				18%	-9.0	-8.7	-11.3

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
1,2-epoxybutane	203-438-2	106-88-7	106887	1447	Reach_679	1853	72	-87.0	2.5E+04	2.9E+04	7.2E+00			1.1E-06	3.5E-07	1.1E-06				15%	-9.0	-8.7	-10.6
610-840-5	226-006-5	5208-93-5	5208935	3052	Reach_2085	1854	220	71.6	9.8E-03	4.7E+00	2.8E+05			1.1E-06	1.1E-07	3.5E-07				14%	-8.7	-8.7	-10.9
617-500-5	205-187-4	135-37-5	135375	5673	Reach_1130	1855	221	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				17%	-8.1	-8.7	-10.3
3-chloro-p-tolyl isocyanate	611-435-6	56962-04-0	56962040	3217	Reach_4359	1856	207	56.4	4.0E-01	1.3E+03	1.1E+03			1.1E-06	3.5E-08	1.1E-07				15%	-8.9	-8.7	-10.2
600-261-6	604-776-7	151213-15-9	151213159	2018	Reach_4163	1857	389	321.2	5.3E-12	1.0E+02	1.2E+01		5.32	3.5E-07	1.1E-07	3.5E-07				16%	-7.8	-8.7	-10.6
2,2-bis[[(1-oxopentyl)oxy]methyl]propane-1,3-diyl divalerate	239-937-7	15834-04-5	15834045	2060	Reach_2402	1858	473	150.1	1.2E-06	3.4E-02	5.5E+06			1.1E-06	1.1E-07	3.5E-07				21%	-8.3	-8.7	-10.0
diethyl sulphate	200-589-6	64-67-5	64675	3442	Reach_73	1859	154	37.8	3.2E+01	2.0E+04	1.4E+01			3.5E-06	1.1E-06	3.5E-06				14%	-8.9	-8.7	-10.5
1-chlorobutane	203-696-6	109-69-3	109693	261	Reach_785	1860	93	-85.2	1.2E+04	6.9E+02	3.6E+02			2.3E-08	3.5E-08	1.1E-07				23%	-9.0	-8.7	-11.2
eugenol	202-589-1	97-53-0	97530	1057	Reach_480	1861	164	60.6	1.3E+00	2.5E+02	5.4E+02	10		7.5E-07	3.5E-07	1.1E-06				15%	-8.9	-8.7	-10.3
2,4-difluoroaniline	242-615-9	18835-33-1	18835331	2210	Reach_2469	1862	365	114.8	2.9E-04	3.1E-08	9.3E+12		0	1.1E-06	1.1E-07	3.5E-07				14%	-8.1	-8.7	-10.7
trimethoxy(methyl)silane	214-685-0	1185-55-3	1185553	1672	Reach_1666	1863	136	-60.0	4.5E+03	1.9E+04	2.1E-01			1.1E-06	3.5E-07	1.1E-06				15%	-9.0	-8.7	-10.5
(S)-(+)-2-(2-Chlorophenyl)-2-hydroxyacetic acid	700-307-6	52950-19-3	52950193	5918	Reach_4853	1864	373	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.4	-8.7	-10.3
(2E)-3,7-dimethylocta-2,6-dien-1-amine	624-182-1	4187-38-6	4187386	2885	Reach_4579	1865	135	17.6	2.7E+01	1.5E+03	1.1E+02		4.7	3.5E-07	3.5E-08	1.1E-07				15%	-8.9	-8.7	-10.4
N-[4-(aminocarbonyl)phenyl]-4-nitrobenzamide	610-886-6	52688-08-1	52688081	3068	Reach_4338	1866	197	43.6	3.4E-01	1.2E+02	7.8E+02			1.1E-06	1.1E-07	3.5E-07				14%	-7.6	-8.7	-10.8
3,9-bis(2,4-di-tert-butylphenoxy)-2,4,8,10-tetraoxa-3,9-diphos	247-952-5	26741-53-7	26741537	2485	Reach_2591	1867	605	257.0	3.9E-11	1.6E-06	7.9E+10			3.5E-07	1.1E-07	3.5E-07				24%	-8.8	-8.7	-9.2
4,5-dihydroxy-1,3-dimethylimidazolidin-2-one	223-496-2	3923-79-3	3923793	2836	Reach_2002	1868	146	85.6	1.8E-03	9.9E+05	1.0E-03	13.5	15.4	1.1E-06	1.1E-07	3.5E-07				14%	-7.4	-8.7	-10.8
1,3,5-triallyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	606-251-8	1917-44-8	1917448	2224	Reach_4201	1869	249	214.7	2.7E-08	8.4E+01	4.8E+03			1.1E-06	1.1E-07	3.5E-07				18%	-8.0	-8.7	-10.3
5-(4-hydroxyphenyl)imidazolidine-2,4-dione	239-106-9	15022-08-9	15022089	2008	Reach_2375	1870	142	-74.2	7.7E+02	1.5E+04	8.5E+01			1.1E-06	1.1E-07	3.5E-07				14%	-7.6	-8.7	-10.6
N-lauroylsarcosine	202-608-3	97-78-9	97789	4172	Reach_488	1871	271	149.4	5.1E-05	8.9E+00	1.3E+04	3.3		1.1E-06	1.1E-07	3.5E-07				14%	-8.2	-8.7	-10.7
3-cyclopentyl-1H-indole-6-carboxylic acid	936-788-6	1307233-94-8	1307233948	1841	Reach_5143	1872	401	254.5	5.8E-11	1.5E+01	5.5E+03			1.1E-06	1.1E-07	3.5E-07				14%	-8.0	-8.7	-10.6
608-748-5	205-138-7	134-32-7	134327	430	Reach_1127	1873	143	70.9	1.5E-01	8.1E+01	1.8E+02			8.3E-09	1.1E-07	3.5E-07				20%	-8.1	-8.7	-10.0
2,4-dichloro-1,3-dinitro-5-(trifluoromethyl)benzene	249-420-8	29091-09-6	29091096	2557	Reach_2627	1874	305	121.5	3.6E-03	1.0E+01	7.6E+03			1.1E-06	3.5E-08	1.1E-07				16%	-8.9	-8.7	-10.6
phthaloyl dichloride	201-660-4	86-28-2	86282	3903	Reach_301	1875	195	103.1	4.7E-03	9.7E+00	1.9E+04			1.1E-06	3.5E-08	1.1E-07				14%	-8.9	-8.7	-10.6
isooctadecyl palmitate	614-477-3	6842-62-2	6842622	3515	Reach_4398	1876	239	91.9	2.3E-02	5.4E+00	2.2E+05			1.1E-06	3.5E-08	1.1E-07				24%	-8.9	-8.7	-7.8
isodecyl diphenyl phosphate	249-828-6	29761-21-5	29761215	588	Reach_2630	1877	390	88.9	6.3E-06	9.1E-03	1.9E+07			1.6E-08	1.1E-07	3.5E-07				24%	-8.0	-8.7	-9.4
6-amino-5-formamido-1,3-dimethyluracil	208-793-7	541-85-5	541855	686	Reach_1342	1878	128	-42.1	4.6E+02	5.7E+02	1.4E+02	0	0	5.5E-07	3.5E-07	1.1E-06				14%	-7.4	-8.7	-10.8
1,3-dichloro-5-isocyanatobenzene	690-920-4	494799-38-1	494799381	2982	Reach_4662	1879	257	125.5	5.5E-04	1.6E+01	5.8E+04			1.1E-06	1.1E-07	3.5E-07				20%	-9.0	-8.7	-10.2
4-chloro-α,α,α-trifluorotoluene	202-681-1	98-56-6	98566	4187	Reach_513	1880	181	-29.9	9.1E+02	4.1E+01	4.0E+03			1.1E-07	1.1E-08	3.5E-08				23%	-9.0	-8.7	-11.3
2-amino-4-nitrophenol	202-767-9	99-57-0	99570	4206	Reach_531	1881	154	109.7	2.0E-03	6.5E+03	9.8E+00	6.61	11.5	3.5E-06	1.1E-07	3.5E-07				14%	-7.7	-8.7	-10.8
O,O,O-triphenyl phosphorothioate	209-909-9	597-82-0	597820	3288	Reach_1401	1882	342	86.2	3.4E-05	1.1E-01	3.0E+06			3.5E-07	3.5E-08	1.1E-07				21%	-8.5	-8.7	-10.0
4-[(6-amino-1-hydroxy-3-sulpho-2-naphthyl)azo]-3-hydroxy-7-(	700-424-2	6872-10-2	6872102	1286	Reach_4897	1883	231	98.7	3.2E-02	1.1E+02	1.3E+04	0	0	3.5E-07	1.1E-07	3.5E-07				16%	-7.8	-8.7	-10.6
(6R-trans)-7-amino-8-oxo-3-[[(1,2,5,6-tetrahydro-2-methyl-5,6-	212-338-8	791-28-6	791286	95	Reach_1547	1884	278	87.0	3.8E-05	4.2E+00	7.4E+02	0	0	6.3E-09	3.5E-09	1.1E-08				16%	-7.6	-8.7	-10.6
607-301-1	700-490-2	36635-56-0	36635560	2772	Reach_4911	1885	213	163.7	4.0E-05	1.2E+03	1.3E-01		0	1.1E-06	1.1E-07	3.5E-07				16%	-7.8	-8.7	-10.6
2'-[2,4-dichloro-5-(1-methylethoxy)phenyl]-2,2-dimethylpropio	257-027-8	51167-18-1	51167181	3028	Reach_2769	1886	319	179.0	5.7E-06	5.1E-01	2.4E+04			1.1E-06	1.1E-07	3.5E-07				16%	-8.6	-8.7	-10.5
thiodiglycol	229-662-0	6642-31-5	6642315	3474	Reach_2200	1887	155	137.1	1.0E-03	9.0E+03	5.5E-02			1.1E-06	1.1E-07	3.5E-07				14%	-7.8	-8.7	-10.7
608-356-4	613-147-6	63141-09-3	63141093	3395	Reach_4382	1888	119	-23.3	1.7E+03	1.2E+04	6.0E+00			1.1E-06	3.5E-07	1.1E-06				16%	-9.0	-8.7	-10.0
(1R)-1-Phenylpropan-1-amine	264-133-8	63422-71-9	63422719	3400	Reach_2857	1889	319	260.5	2.2E-11	5.1E+02	5.6E+00		15.6	3.5E-06	3.5E-07	1.1E-06				16%	-9.0	-8.7	-10.0
2-dibutylaminoethanol	203-057-1	102-81-8	102818	1354	Reach_599	1890	173	29.1	1.7E+00	2.4E+03	1.0E+02	15	4.1	1.1E-06	3.5E-07	1.1E-06				14%	-9.0	-8.7	-10.6
623-635-0	256-283-8	46830-22-2	46830222	5893	Reach_2758	1891	270	0.0												16%	-9.0	-8.7	-10.0
(1R)-1-(4-methylphenyl)ethanamine	632-902-0	82796-69-8	82796698	3837	Reach_4599	1892	151	18.8	1.6E+01	6.1E+03	2.1E+01		4.81	1.1E-06	1.1E-07	3.5E-07				16%	-9.0	-8.7	-10.0
N-(3-aminopropyl)-N-dodecylpropane-1,3-diamine	219-145-8	2372-82-9	2372829	554	Reach_1788	1893	300	137.5	2.0E-04	2.4E+02	2.9E+04		3	4.0E-07	1.1E-07	3.5E-07				18%	-8.2	-8.7	-10.4
salicylaldehyde	201-961-0	90-02-8	90028	998	Reach_356	1894	122	42.6	3.0E+01	8.8E+03	1.0E+02	8.4		1.6E-06	1.1E-06	3.5E-06				14%	-9.0	-8.7	-10.5
(2R)-3-cyano-2-hydroxy-N,N,N-trimethylpropan-1-aminium chl	700-244-4	5895-82-9	5895829	3263	Reach_4819	1895	176	5.1	3.1E+03	0.0E+00	1.8E+02									18%	-8.4	-8.7	-10.4
4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl	218-760-9	2226-96-2	2226962	2327	Reach_1775	1896	173	102.4	2.0E-04	1.8E+06	3.6E+00	16		1.1E-06	3.5E-07	1.1E-06				14%	-7.7	-8.7	-10.7
3-hydroxy-2-(hydroxymethyl)-2-methylpropionaldehyde	242-393-3	18516-18-2	18516182	2194	Reach_2464	1897	118	33.8	3.3E-01	3.1E+05	4.7E-02	14.4		3.5E-06	1.1E-06	3.5E-06				14%	-7.9	-8.7	-10.7
tert-butyl acrylate	216-768-7	1663-39-4	1663394	2103	Reach_1706	1898	128	-51.4	1.7E+03	2.6E+03	1.2E+02			1.1E-06	3.5E-07	1.1E-06				16%	-9.0	-8.7	-10.7
4-amino-2-methylpyrimidine-5-methylamine	222-483-9	3490-06-0	3490060	2718	Reach_1968	1899	195	69.6	2.8E-01	3.8E+02	2.8E+01		4.14	1.1E-06	1.1E-07	3.5E-07				16%	-7.8	-8.7	-10.6
l-p-mentha-1(6),8-dien-2-one	219-348-1	2421-28-5	2421285	2378	Reach_1803	1900	322	188.4	3.1E-07	1.7E+01	2.0E+03			1.1E-06	1.1E-07	3.5E-07				17%	-9.0	-8.7	-10.0
(2S,3S,3aR,9aS)-3-hydroxy-2-(hydroxymethyl)-7-methyl-	619-693-1	159276-62-7	159276627	2067	Reach_4537	1901	312	23.3	9.0E-02	9.8E+00	2.1E+04	12.8		1.1E-06	1.1E-07	3.5E-07				14%	-7.6	-8.7	-10.8
citronellal	203-376-6	106-23-0	106230	1432	Reach_660	1902	154	-28.3	3.4E+01	2.9E+02	3.4E+03			1.1E-06	3.5E-07	1.1E-06				16%	-9.0	-8.7	-10.2
anisole	202-876-1	100-66-3	100663	136	Reach_567	1903	108	-41.2	4.5E+02	3.3E+03	1.2E+02			5.9E-07	3.5E-07	1.1E-06				16%	-9.0	-8.7	-10.2
4-hydroxybenzenesulphonic acid	202-691-6	98-67-9	98679	4190	Reach_516	1904	174	128.7	4.4E-05	2.5E+04	2.2E-02	0.96		1.1E-05	1.1E-06	3.5E-06				14%	-7.5	-8.7	-10.6
4,11-dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione	696-317-2	174489-76-0	174489760	2138	Reach_4713	1905	328	122.5	4.3E-04	7.4E+00	3.5E+03	0	0	1.1E-06	1.1E-07	3.5E-07				19%	-8.4	-8.7	-10.3
dimethyl adipate	211-020-6	627-93-0	627930	3378	Reach_1460	1906	174	-71.5	9.2E+01	1.3E+04	2.5E+01			3.5E-06	3.5E-07	1.1E-06				14%	-8.9	-8.7	-10.5
retinyl palmitate	201-228-5	79-81-2	79812	3784	Reach_250	1907	525	222.0	1.5E-07	1.1E-08	3.2E+15			1.1E-06	1.1E-07	3.5E-07				24%	-9.0	-8.7	-7.9
ethyldimethylamine	209-940-8	598-56-1	598561	741	Reach_1404	1908	73	-96.5	6.6E+04	1.1E+05	3.4E+00		4	5.1E-08	1.1E-06	3.5E-06				22%	-9.0	-8.7	-10.5
606-964-4	201-153-8	78-88-6	78886	903	Reach_214	1909	111	-82.7	6.5E+03	2.3E+03	2.6E+02	0	0	8.2E-08	1.1E-08	3.5E-08				16%	-8.0	-8.7	-10.6
3,7,7-trimethylbicyclo[4.1.0]hept-3-ene	236-719-3	13466-78-9	13466789	434	Reach_2337	1910	136	-13.6	2.8E+02	2.8E+01	4.1E+04			3.2E-07	3.5E-08	1.1E-07				22%	-9.0	-8.7	-11.2
disodium 4,4'-bis[[6-anilino-4-[(2-hydroxyethyl)methylamino]-1	237-600-9	13863-31-5	13863315	1191	Reach_2350	1911	901	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.4	-8.7	-10.4
3,3'-(ethylenediimino)bispropiononitrile	607-936-4	26447-85-8	26447858	2469	Reach_4254	1912	254	131.8	2.1E-05	4.4E+02	7.1E+01			1.1E-06	1.1E-07	3.5E-07				14%	-7.6	-8.7	-10.9
potassium dimethyldithiocarbamate	204-875-1	128-03-0	128030	1187	Reach_1104	1913	159	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.4	-8.7	-10.4
2-ethyl-N,N-bis(2-ethylhexyl)hexylamine	278-575-4	76918-62-2	76918622	6033	Reach_2948	1914	342	0.0	0.0E+00	0.0E+00	0.0E+00		0	0.0E+00	0.0E+00	0.0E+00				23%	-8.8	-8.7	-9.9
isovaleric acid	207-975-3	503-74-2	503742	657	Reach_1302	1915	102	3.6	1.5E+02	4.6E+04	3.1E+01	4.9		3.5E-07	3.5E-07	1.1E-06				16%	-8.6	-8.7	-10.5
2-cyano-2-[2,3-dihydro-3-(tetrahydro-2,4,6-trioxo-5(2H)-pyrim	278-388-8	76199-85-4	76199854	3703	Reach_2947	1916	337	349.8	7.9E-18	2.6E+03	7.9E-02	1.78	5.29	1.1E-06	1.1E-07	3.5E-07				14%	-7.5	-8.7	-10.8
1,3-dioxepane	208-015-6	505-65-7	505657	3010	Reach_1309	1917	102	-52.3	1.8E+03	6.7E+04	4.7E+00			3.5E-07	1.1E-07	3.5E-07				16%	-9.0	-8.7	-10.0
(trimethoxysilyl)methyl prop-2-enoate	618-109-2	88069-93-6	88069936	3946	Reach_4486	1918	216	67.0	5.4E-02	1.5E+01	1.4E+04			3.5E-07	1.1E-07	3.5E-07				14%	-8.0	-8.7	-10.9
didodecyl fumarate	219-280-2	2402-58-6	2402586	2365	Reach_1794	1919	453	94.6	5.4E-06	2.7E-06	1.0E+12			1.1E-06	1.1E-07	3.5E-07				24%	-8.9	-8.7	-9.2
610-122-1	696-441-7	256473-05-9	256473059	2442	Reach_4717	1920	251	56.3	8.0E-01	2.2E+01	5.8E+03			3.5E-07	1.1E-07	3.5E-07				14%	-7.6	-8.7	-10.8
ursodeoxycholic acid	204-879-3	128-13-2	128132	1816	Reach_1107	1921	393	216.4	5.1E-10	4.3E+01	1.1E+05	4.9		1.1E-06	1.1E-07	3.5E-07				15%	-8.1	-8.7	-10.6
pentasodium bis[5-[(4-amino-6-chloro-1,3,5-triazin-2-yl)amino	279-317-3	79828-43-6	79828436	6041	Reach_2957	1922	1385	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.4	-8.7	-10.4
1,3-bis(1-isocyanato-1-methylethyl)benzene	220-474-4	2778-42-9	2778429	2517	Reach_1865	1923	244	107.0	1.4E-02	1.5E+02	5.5E+04			1.1E-06	1.1E-07	3.5E-07				17%	-8.9	-8.7	-10.5
diethyl ether	200-467-2	60-29-7	60297	750	Reach_57	1924	74	-101.2	7.2E+04	4.8E+04	1.1E+01			3.0E-08	1.1E-07	3.5E-07				23%	-9.0	-8.7	-10.8
2'-anilino-6'-[ethyl(3-methylbutyl)amino]-3'-methylspiro[isober	274-641-1	70516-41-5	70516415	3563	Reach_2918	1925	519	289.0	2.4E-13	4.6E-06	5.2E+08		10.2	1.1E-06	1.1E-07	3.5E-07				16%	-7.8	-8.7	-10.5
604-351-6	603-567-8	132335-47-8	132335478	5666	Reach_4126	1926	401	0.0												20%	-8.6	-8.7	-10.2
furfurylamine	805-957-5	848655-78-7	848655787	3879	Reach_5071	1927	194	148.3	1.5E-04	5.0E+03	1.5E+00		9.89	3.5E-07	1.1E-07	3.5E-07				14%	-9.0	-8.7	-10.3

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
propane-1,3-diol	207-997-3	504-63-2	504632	660	Reach_1306	1928	76	-19.7	2.8E+00	1.4E+06	1.9E-01	15.3		4.3E-06	1.1E-06	3.5E-06				14%	-7.9	-8.7	-10.7
3-(methylamino)propane-1,2-diol	254-809-0	40137-22-2	40137222	2853	Reach_2729	1929	105	16.2	2.8E+00	1.0E+06	1.6E-02	14.1	4.5	3.5E-06	1.1E-06	3.5E-06				14%	-8.0	-8.7	-10.8
2,9-bis(2-phenylethyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoquinol	266-564-7	67075-37-0	67075370	3484	Reach_2884	1930	599	349.8	1.6E-23	3.3E-07	3.8E+08		12.9	1.1E-07	3.5E-09	1.1E-08				19%	-8.5	-8.7	-10.3
3',4'-dichloro-5-fluorobiphenyl-2-amine	203-360-9	106-09-2	106092	1427	Reach_655	1931	286	183.8	1.9E-08	2.1E+00	5.4E+02		5.8	1.1E-06	3.5E-07	1.1E-06				16%	-8.2	-8.7	-10.7
609-920-2	243-473-0	20030-30-2	20030302	2248	Reach_2487	1932	138	4.7	5.1E+01	4.1E+03	3.8E+02			1.1E-06	3.5E-07	1.1E-06				16%	-7.8	-8.7	-10.6
perhydroazepine	203-875-9	111-49-9	111499	304	Reach_860	1933	99	-13.7	9.3E+02	6.6E+04	4.8E+01		3	3.1E-09	1.1E-07	3.5E-07				23%	-9.0	-8.7	-9.9
3,5-dichlorobenzoyl chloride	220-813-6	2905-62-6	2905626	2556	Reach_1882	1934	209	54.1	1.2E+00	1.0E+01	5.4E+02			1.1E-07	1.1E-08	3.5E-08				20%	-9.0	-8.7	-10.3
2-amino-5-nitrophenol	204-515-3	122-01-0	122010	1741	Reach_1024	1935	175	32.7	1.6E+01	3.3E+02	1.2E+02			1.1E-07	1.1E-08	3.5E-08				14%	-7.7	-8.7	-10.9
3-aminopropane-1,2-diol	210-475-8	616-30-8	616308	3343	Reach_1430	1936	91	24.6	3.7E+00	1.0E+06	5.6E-03	14.1	4.9	3.5E-06	1.1E-06	3.5E-06				14%	-8.0	-8.7	-10.8
dimethyl 2-aminoterephthalate	226-364-2	5372-81-6	5372816	683	Reach_2103	1937	209	30.4	1.6E-01	3.8E+03	1.3E+02		12	7.1E-07	1.1E-07	3.5E-07				15%	-8.1	-8.7	-10.7
triisotridecyl benzene-1,2,4-tricarboxylate	276-594-2	72361-35-4	72361354	3603	Reach_2936	1938	757	312.9	5.3E-15	9.2E-14	9.1E+18			1.1E-06	1.1E-07	3.5E-07				24%	-9.0	-8.7	-6.3
isodecyl diphenyl phosphite	247-777-4	26544-23-0	26544230	2476	Reach_2587	1939	374	154.8	7.0E-06	5.8E-03	3.3E+08			3.5E-07	1.1E-07	3.5E-07				23%	-8.3	-8.7	-9.4
2-ethylhexanoyl chloride	212-081-1	760-67-8	760678	3697	Reach_1531	1940	163	-17.7	5.8E+01	2.0E+01	2.5E+02			3.5E-07	1.1E-07	3.5E-07				21%	-9.0	-8.7	-11.0
Methyl 3-[(2,2-dimethylbutanoyl)thio]propanoate	620-518-6	938063-63-9	938063639	4084	Reach_4574	1941	218	53.6	4.5E-01	3.9E+02	1.3E+02			3.5E-06	3.5E-07	1.1E-06				14%	-9.0	-8.7	-10.6
619-529-9	210-787-4	623-33-6	623336	5956	Reach_1448	1942	140	0.0	0.0E+00	0.0E+00	0.0E+00		0	0.0E+00	0.0E+00	0.0E+00				16%	-7.9	-8.7	-10.6
1,6,7,8,9,14,15,16,17,17,18,18-dodecachloropentacyclo[12.2.1	236-948-9	13560-89-9	13560899	1892	Reach_2341	1943	654	206.5	9.4E-08	4.8E-06	1.9E+11			3.5E-08	3.5E-09	1.1E-08				24%	-9.0	-8.7	-9.1
3-diethylaminophenol	202-090-9	91-68-9	91689	4019	Reach_379	1944	165	60.5	1.1E-01	4.0E+02	2.1E+02	9.9	9.9	3.5E-06	1.1E-07	3.5E-07				14%	-7.9	-8.7	-10.8
acetone oxime	204-820-1	127-06-0	127060	410	Reach_1095	1945	73	-70.1	1.6E+02	5.6E+04	1.6E+01	12.5		2.8E-07	3.5E-07	1.1E-06				16%	-9.0	-8.7	-10.3
N-(3-(trimethoxysilyl)propyl)ethylenediamine	217-164-6	1760-24-3	1760243	2145	Reach_1718	1946	222	68.7	4.7E-01	2.9E+05	2.1E-02		4.34	3.5E-06	1.1E-06	3.5E-06				14%	-8.0	-8.7	-10.8
1-amino-1-deoxy-D-glucitol	227-577-3	5894-79-1	5894791	3261	Reach_2143	1947	178	33.9	1.2E+00	4.8E+03	1.0E+01	5.9		3.5E-06	3.5E-07	1.1E-06				14%	-7.7	-8.7	-10.8
4-chlorobenzoyl chloride	619-326-5	98210-99-2	98210992	4180	Reach_4513	1948	545	349.8	6.2E-23	4.4E-03	6.8E-02			1.1E-06	1.1E-08	3.5E-08				19%	-9.0	-8.7	-10.2
chenodeoxycholic acid	207-481-8	474-25-9	474259	2966	Reach_1289	1949	393	216.4	5.1E-10	4.3E+01	1.1E+05	4.9		1.1E-06	1.1E-07	3.5E-07				15%	-8.1	-8.7	-10.6
N-(hydroxymethyl)methacrylamide	213-086-1	923-02-4	923024	4030	Reach_1592	1950	115	80.2	2.7E+03	2.6E+05	5.5E-02	13.3	15.3	3.5E-06	3.5E-07	1.1E-06				14%	-7.6	-8.7	-10.8
taurine	608-544-6	3082-64-2	3082642	2613	Reach_4277	1951	135	11.3	2.7E+01	1.5E+03	9.5E+01		4.7	3.5E-07	3.5E-08	1.1E-07				14%	-7.7	-8.7	-10.8
615-497-5	249-070-6	28535-81-1	28535811	2535	Reach_2620	1952	505	202.4	2.7E-08	2.0E-01	4.0E+05									18%	-8.4	-8.8	-10.4
propyl 4-hydroxybenzoate	202-307-7	94-13-3	94133	109	Reach_412	1953	180	71.8	4.1E-02	4.7E+02	9.5E+02	8.5		6.6E-07	3.5E-07	1.1E-06				15%	-8.9	-8.8	-10.6
ethyl 2-cyanoacrylate	230-391-5	7085-85-0	7085850	3571	Reach_2224	1954	125	-9.3	3.9E+01	5.6E+03	2.6E+01			3.5E-06	3.5E-07	1.1E-06				14%	-9.0	-8.8	-10.5
2-(2-naphthyloxy)ethanol	202-228-8	93-20-9	93209	4065	Reach_401	1955	188	94.5	5.7E-04	1.5E+03	1.9E+02	14.8		1.1E-06	3.5E-08	1.1E-07				15%	-7.9	-8.8	-10.8
methyl vinyl ether	203-475-4	107-25-5	107255	1456	Reach_702	1956	58	-116.0	2.0E+05	4.5E+04	2.6E+00			1.1E-06	1.1E-07	3.5E-07				17%	-9.2	-8.8	-11.0
6-tert-butyl-m-cresol	201-842-3	88-60-8	88608	3961	Reach_327	1957	164	51.9	1.1E+00	5.5E+02	9.3E+03	10.8		3.5E-06	3.5E-07	1.1E-06				15%	-9.0	-8.8	-10.6
N,N'-bis(1,4-dimethylpentyl)-p-phenylenediamine	221-375-9	3081-14-9	3081149	2612	Reach_1913	1958	305	112.7	1.1E-03	4.3E-02	2.0E+06		7.7	1.1E-06	1.1E-07	3.5E-07				19%	-8.9	-8.8	-10.4
propane-1,2,3-triyl 3,5,5-trimethylhexanoate	260-257-1	56554-53-1	56554531	3202	Reach_2817	1959	513	111.4	9.5E-06	5.6E-05	1.3E+10			1.1E-06	1.1E-07	3.5E-07				23%	-8.8	-8.8	-9.4
ethanethiol	200-837-3	75-08-1	75081	849	Reach_128	1960	62	-102.1	6.9E+04	9.1E+03	1.9E+01	10.7		2.8E-09	3.5E-07	1.1E-06				24%	-9.1	-8.8	-11.1
1-benzyl-1,2-dihydro-3H-indazol-3-one, sodium salt	236-138-5	13185-09-6	13185096	5663	Reach_2325	1961	247	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.5	-8.8	-10.4
1-[4-(trans-4-propylcyclohexyl)phenyl]pentan-1-one	601-770-6	121315-20-6	121315206	1725	Reach_4103	1962	352	264.8	2.0E-14	1.3E+03	3.3E-05			1.1E-06	3.5E-07	1.1E-06				23%	-8.4	-8.8	-9.8
3,4-dichlorotoluene	700-475-0	145783-14-8	145783148	1988	Reach_4907	1963	268	144.6	6.8E-04	2.0E+01	1.5E+03			3.5E-07	3.5E-08	1.1E-07				24%	-9.1	-8.8	-10.7
2-methylbutan-2-ol	252-173-9	34730-59-1	34730591	5853	Reach_2682	1964	190	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				21%	-9.0	-8.8	-10.0
p-phenylbenzonitrile	220-860-2	2920-38-9	2920389	2561	Reach_1885	1965	179	86.5	1.3E-02	1.9E+01	2.0E+03			3.5E-07	3.5E-08	3.5E-08				16%	-9.0	-8.8	-10.5
trometamol	201-064-4	77-86-1	77861	3739	Reach_187	1966	121	80.8	3.0E-04	1.0E+06	2.8E-02	13.9	5.9	3.5E-06	1.1E-06	3.5E-06				14%	-7.7	-8.8	-10.8
2,9-bis(p-methoxybenzyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoqui	280-472-4	83524-75-8	83524758	3848	Reach_2967	1967	631	349.8	3.4E-24	9.7E-07	5.8E+07		13	1.1E-07	3.5E-09	1.1E-08				19%	-8.6	-8.8	-10.4
(Z)-N-9-octadecenylpropane-1,3-diamine	230-528-9	7173-62-8	7173628	3589	Reach_2229	1968	325	142.1	6.5E-05	1.7E-04	3.0E+07		3.3	1.1E-06	1.1E-07	3.5E-07				22%	-8.8	-8.8	-10.5
fluorene	201-695-5	86-73-7	86737	973	Reach_302	1969	166	63.7	4.4E-02	4.1E+00	1.0E+04			8.9E-08	3.5E-08	3.5E-08				20%	-9.0	-8.8	-10.0
dimethoxymethane	203-714-2	109-87-5	109875	268	Reach_795	1970	76	-95.4	5.5E+04	2.4E+05	6.5E-01			9.8E-07	1.1E-07	3.5E-07				15%	-9.1	-8.8	-10.5
N-[4-(1,1,1,2,3,3,3-heptafluoropropan-2-yl)-2-methylphenyl]-N	609-338-9	371771-07-2	371771072	2793	Reach_4299	1971	541	275.1	2.9E-15	8.9E-04	6.0E+05	13.2		1.1E-06	1.1E-07	3.5E-07				19%	-8.0	-8.8	-10.3
606-050-5	212-161-6	766-09-6	766096	874	Reach_1542	1972	113	-26.2	1.3E+03	7.1E+04	7.8E+01	0		6.2E-07	1.1E-07	1.1E-06				21%	-8.1	-8.8	-10.2
12H-phthaloperin-12-one	202-549-3	96-98-0	96980	4159	Reach_474	1973	181	118.5	4.5E-03	1.3E+03	1.7E+02		0	3.5E-06	1.1E-07	3.5E-07				16%	-8.0	-8.8	-10.6
3-methylpyrazole	215-925-7	1453-58-3	1453583	1985	Reach_1683	1974	82	17.6	2.8E+01	2.6E+04	4.1E+00		10.6	3.5E-07	3.5E-08	1.1E-07				16%	-7.7	-8.8	-10.7
bis[2-[2-(1-methylethyl)-3-oxazolidinyl]ethyl] hexan-1,2-diylbis(	261-879-6	59719-67-4	59719674	3284	Reach_2841	1975	487	214.9	1.9E-08	3.4E+01	8.3E+02	11.2	7.75	1.1E-06	1.1E-07	3.5E-07				15%	-8.0	-8.8	-10.7
2-[[(4-methoxyphenyl)methylhydrazono]methyl]-1,3,3-trimeth	261-448-2	58798-47-3	58798473	5941	Reach_2832	1976	381	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.5	-8.8	-10.4
arginine	200-811-1	74-79-3	74793	3644	Reach_107	1977	174	296.8	1.8E-06	4.4E+04	1.0E-04	1.86	1.9	3.5E-06	3.5E-07	1.1E-06				14%	-7.5	-8.8	-10.9
propane-1,2-diyl diacetate	210-817-6	623-84-7	623847	3367	Reach_1450	1978	160	-94.6	7.7E+01	5.0E+04	6.6E+00			3.5E-06	3.5E-07	1.1E-06				14%	-9.0	-8.8	-10.7
620-464-3	700-287-9	877179-04-9	877179049	3939	Reach_4842	1979	256	122.9	9.7E-04	1.7E+00	2.1E+04		11	3.5E-07	1.1E-08	3.5E-08				16%	-8.0	-8.8	-10.7
2-amino-4-chloro-6-nitrophenol	234-234-1	10605-40-0	10605400	1426	Reach_2302	1980	171	-43.8	6.4E+02	1.7E+02	5.2E+03			1.1E-07	1.1E-08	3.5E-08				14%	-7.9	-8.8	-10.9
1-bromopropane	203-445-0	106-94-5	106945	203	Reach_684	1981	123	-79.1	1.8E+04	2.2E+03	1.4E+02			2.1E-08	3.5E-07	1.1E-06				23%	-9.1	-8.8	-11.2
stearoyl chloride	700-093-4	176969-34-9	176969349	2150	Reach_4758	1982	176	83.3	3.3E-01	7.7E+03	6.9E+00			1.1E-06	1.1E-07	3.5E-07				23%	-8.9	-8.8	-11.3
2,2'-methylenebis(6-nonyl-p-cresol)	232-092-5	7786-17-6	7786176	3740	Reach_2275	1983	481	251.8	8.3E-13	3.6E-07	1.3E+13	9.67		1.1E-06	1.1E-07	3.5E-07				24%	-9.0	-8.8	-9.1
5-phenyl-o-anisidine	927-913-5	160844-75-7	160844757	2077	Reach_5115	1984	344	197.1	3.9E-07	2.8E-01	4.6E+04		12.9	1.1E-06	1.1E-07	3.5E-07				16%	-8.2	-8.8	-10.7
trifluoroacetic acid	200-929-3	76-05-1	76051	3695	Reach_171	1985	114	-24.0	1.5E+04	1.1E+07	3.2E+00	0.6		3.5E-06	3.5E-07	1.1E-06				14%	-7.8	-8.8	-10.8
methyl octanoate	203-835-0	111-11-5	111115	1538	Reach_844	1986	158	-20.9	6.8E+01	1.2E+02	2.1E+03			1.1E-06	1.1E-07	3.5E-07				16%	-9.1	-8.8	-10.7
di-sec-butylphenol	250-184-3	30414-53-0	30414530	2595	Reach_2645	1987	130	-19.2	2.2E+02	4.2E+04	6.3E-01	10.6		3.5E-06	3.5E-07	1.1E-06				18%	-8.9	-8.8	-10.5
docosyl acrylate	242-182-6	18299-85-9	18299859	2177	Reach_2458	1988	381	134.6	3.2E-05	1.4E-06	1.1E+11			1.1E-06	1.1E-07	3.5E-07				24%	-9.0	-8.8	-9.7
1,1'-(p-tolylimino)dipropan-2-ol	254-075-1	38668-48-3	38668483	2825	Reach_2717	1989	223	106.8	7.8E-05	3.8E+02	1.0E+02	14.6	10.3	1.1E-06	1.1E-07	3.5E-07				14%	-8.1	-8.8	-10.8
604-776-7	209-010-1	552-37-4	552374	5930	Reach_1359	1990	159	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				16%	-7.9	-8.8	-10.6
α,α,α-trifluoro-p-toluidine	207-236-5	455-14-1	455141	2941	Reach_1279	1991	161	9.6	5.5E+01	4.4E+03	1.1E+02		11.4	1.1E-06	3.5E-07	1.1E-06				14%	-8.0	-8.8	-10.8
1,3-dihydroxyacetone	202-494-5	96-26-4	96264	4143	Reach_458	1992	90	16.7	5.9E-01	3.1E+05	1.9E-01	13.3		3.5E-06	1.1E-06	3.5E-06				14%	-8.0	-8.8	-10.8
7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-3,6,8,	253-211-7	36788-39-3	36788393	2777	Reach_2705	1993	430	207.8	4.5E-11	6.1E+02	3.8E-02	14.6		1.1E-06	1.1E-07	3.5E-07				14%	-7.7	-8.8	-11.0
5-[[4-chloro-6-[(3-sulphophenyl)amino]-1,3,5-triazin-2-yl]amin	279-015-1	78952-61-1	78952611	6040	Reach_2955	1994	984	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.5	-8.8	-10.5
4-amino-2-methylpyrimidine-5-carbonitrile	609-474-9	37750-29-1	37750291	2805	Reach_4302	1995	236	125.5	7.6E-04	9.0E+00	1.0E+04		10.7	3.5E-07	1.1E-07	1.1E-07				16%	-7.8	-8.8	-10.7
butyl glycollate	223-664-5	4009-98-7	4009987	5874	Reach_2005	1996	343	0.0												14%	-9.0	-8.8	-10.8
N,N'-(2-chloro-1,4-phenylene)bis[4-[(4-chloro-2-nitrophenyl)az	217-589-7	1897-52-5	1897525	2217	Reach_1733	1997	139	2.9	9.4E+01	6.4E+02	8.7E+01	0		3.5E-07	3.5E-08	1.1E-07				24%	-9.0	-8.8	-7.6
α,α'-propylenedinitrilodi-o-cresol	202-374-2	94-91-7	94917	4116	Reach_419	1998	282	160.4	4.7E-07	9.0E+01	3.3E+02	12.1	8.73	1.1E-06	3.5E-08	1.1E-07				14%	-8.0	-8.8	-10.9
cis-propenylphosphonic acid	605-830-2	178671-69-7	178671697	2156	Reach_4182	1999	404	233.7	5.3E-10	2.7E+03	2.9E-03	0		3.5E-06	3.5E-07	1.1E-06				16%	-7.8	-8.8	-10.7
tetrabutylurea	224-929-8	4559-86-8	4559868	2943	Reach_2048	2000	284	99.7	2.6E-03	1.6E+00	4.9E+05		13.9	3.5E-07	3.5E-08	1.1E-07				20%	-8.9	-8.8	-10.3
609-474-9	700-807-4	134283-49-1	134283491	1877	Reach_4999	2001	167	96.3	7.8E-04	2.1E+04	1.6E+01		0	3.5E-06	3.5E-07	1.1E-06				16%	-8.4	-8.8	-10.7
octylamine	203-916-0	111-86-4	111864	313	Reach_877	2002	129	-9.7	1.3E+02	3.2E+02	6.3E+02		4	5.0E-07	1.1E-07	3.5E-07				17%	-9.1	-8.8	-10.5

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
8-chloro-5,10-dihydro-11H-dibenzo[b,e][1,4]diazepin-11-one	203-242-7	104-83-6	104836	1401	Reach_630	2003	161	3.4	1.2E+01	8.6E+01	2.8E+03			1.1E-07	1.1E-08	3.5E-08				14%	-8.2	-8.8	-10.9
trimethylenediamine	202-288-5	93-92-5	93925	4093	Reach_409	2004	164	-0.2	1.5E+01	1.1E+03	3.2E+02		0	1.1E-06	1.1E-07	3.5E-07				16%	-9.0	-8.8	-10.5
2-hexyldecan-1-ol	219-370-1	2425-77-6	2425776	2381	Reach_1805	2005	242	50.8	2.4E-03	2.6E-02	4.6E+06	15.9		1.1E-06	1.1E-07	3.5E-07				21%	-8.9	-8.8	-10.2
isometheptene	257-484-3	51867-77-7	51867777	3047	Reach_2775	2006	361	224.8	6.5E-10	3.9E+00	3.4E+07			3.5E-08	1.1E-08	1.1E-08				16%	-9.1	-8.8	-10.1
616-378-0	606-356-9	19708-81-7	19708817	2237	Reach_4205	2007	122	-14.1	2.0E+02	4.2E+03	3.3E+00		0	1.1E-06	1.1E-07	3.5E-07				14%	-8.1	-8.8	-10.8
N,N,N',N'-tetramethylhexamethylenediamine	252-772-5	35869-64-8	35869648	2752	Reach_2695	2008	850	349.8	4.0E-33	1.0E-10	5.6E+14		0	1.1E-07	3.5E-09	1.1E-08				16%	-9.1	-8.8	-10.6
2,4-dichlorotoluene	205-970-0	256-96-2	256962	2444	Reach_1217	2009	193	104.5	7.7E-04	1.7E+01	1.1E+04			3.5E-07	3.5E-08	1.1E-07				21%	-9.1	-8.8	-10.7
N,N,N',N'-tetrakis(2-hydroxypropyl)adipamide	260-982-3	57843-53-5	57843535	3238	Reach_2827	2010	377	237.6	2.2E-13	6.4E+03	7.1E-03	14	14.8	1.1E-06	3.5E-07	1.1E-06				14%	-7.6	-8.8	-10.8
methylsilanetriyl triacetate	224-221-9	4253-34-3	4253343	2896	Reach_2023	2011	220	-44.9	1.8E+01	6.6E+03	1.8E+00			3.5E-06	3.5E-07	1.1E-06				14%	-9.0	-8.8	-10.7
2-methylpentane-1,5-diamine	239-556-6	15520-10-2	15520102	2040	Reach_2390	2012	116	13.4	1.3E+02	1.0E+06	1.9E+00		3.28	3.5E-06	3.5E-07	1.1E-06				14%	-9.0	-8.8	-10.8
609-063-4	609-063-4	35113-48-5	35113485	2723	Reach_4288	2013	274	22.8	2.3E-01	1.1E+03	2.9E+01			3.5E-06	3.5E-07	1.1E-06				14%	-9.1	-8.8	-10.8
butyl 2-[[3-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]ca	250-800-0	31778-10-6	31778106	2634	Reach_2657	2014	524	349.8	2.0E-19	1.7E-03	6.5E+07	9.46	15.7	3.5E-07	1.1E-08	3.5E-08				16%	-8.5	-8.8	-10.7
hexahydro-4,7-methano-1H-indenyl acrylate	223-032-9	3699-54-5	3699545	2788	Reach_1984	2015	130	93.4	2.1E-03	5.4E+05	3.2E-02			3.5E-06	1.1E-06	3.5E-06				15%	-9.1	-8.8	-10.5
diphenyl sulphone	204-853-1	127-63-9	127639	1813	Reach_1100	2016	218	113.1	7.3E-02	1.6E+01	4.1E+02			1.1E-06	1.1E-07	3.5E-07				15%	-9.1	-8.8	-10.5
tris(2-ethylhexyl) 2-(acetyloxy)propane-1,2,3-tricarboxylate	205-617-0	144-15-0	144150	1971	Reach_1193	2017	571	184.6	1.4E-08	3.2E-05	9.1E+09			1.1E-06	1.1E-07	3.5E-07				23%	-8.8	-8.8	-9.4
N,N'-hexane-1,6-diylbis[3-(3,5-di-tert-butyl-4-hydroxyphenylpr	245-442-7	23128-74-7	23128747	2345	Reach_2527	2018	637	349.8	4.2E-21	5.7E-07	4.1E+09	11.7	13.9	1.1E-06	1.1E-07	3.5E-07				23%	-8.7	-8.8	-9.4
ethylenebis(oxyethylene) bis[3-(5-tert-butyl-4-hydroxy-m-tolyl)	253-039-2	36443-68-2	36443682	2767	Reach_2699	2019	587	274.3	1.5E-14	3.3E-04	1.6E+08	11.6		1.1E-06	1.1E-07	3.5E-07				22%	-8.3	-8.8	-9.6
2-fluorobenzoyl chloride	231-397-0	7531-52-4	7531524	3666	Reach_2259	2020	114	96.0	1.1E-01	1.6E+06	1.1E-01			3.5E-06	1.1E-06	3.5E-06				14%	-9.1	-8.8	-10.4
2-(2-oxoimidazolidin-1-yl)ethyl methacrylate	289-214-5	86261-90-7	86261907	3902	Reach_2989	2021	198	108.6	5.1E-03	2.4E+04	2.6E+00	13.5	14.5	3.5E-06	3.5E-07	1.1E-06				14%	-7.7	-8.8	-10.8
2-ethylaminoethanol	203-797-5	110-73-6	110736	282	Reach_826	2022	89	-23.6	5.9E+01	1.0E+06	2.2E-01	15	4	5.0E-07	1.1E-06	3.5E-06				15%	-8.9	-8.8	-10.7
manganese, 4-[(5-chloro-4-methyl-2-sulfophenyl)azo]-3-hydro	226-102-7	5280-66-0	5280660	5916	Reach_2089	2023	476	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.5	-8.8	-10.5
triethoxyoctylsilane	220-941-2	2943-75-1	2943751	2567	Reach_1891	2024	276	53.5	1.9E-01	7.9E+00	1.7E+04			1.1E-06	1.1E-07	3.5E-07				16%	-9.1	-8.8	-10.3
4-[(2,5-dichlorophenyl)azo]-N-(2,3-dihydro-2-oxo-1H-benzimid	230-258-1	6992-11-6	6992116	1287	Reach_2217	2025	492	332.1	8.1E-18	1.2E-03	6.2E+07	9.27	15.7	3.5E-07	3.5E-08	3.5E-08				16%	-8.5	-8.8	-10.7
3-methyl-1-(2,6,6-trimethylcyclohex-1-en-1-yl)penta-1,4-dien-3	259-487-5	55117-15-2	55117152	3162	Reach_2805	2026	179	8.7	2.7E+01	9.6E+01	4.4E+03			3.5E-07	3.5E-08	1.1E-07				18%	-8.9	-8.8	-10.5
605-444-4	605-444-4	166524-64-7	166524647	2104	Reach_4174	2027	158	81.8	9.0E-01	7.5E+04	8.3E-01		13.2	3.5E-07	3.5E-08	1.1E-07				16%	-7.9	-8.8	-10.7
propylidynetrimethyl trimethacrylate	221-950-4	3290-92-4	3290924	2669	Reach_1942	2028	338	-8.5	1.8E-02	2.3E+01	3.2E+04			3.5E-06	3.5E-07	1.1E-06				16%	-9.1	-8.8	-10.7
bis(2-ethylhexyl) fumarate	205-448-2	141-02-6	141026	1931	Reach_1155	2029	341	28.9	2.6E-01	9.8E-03	8.7E+07			3.5E-07	3.5E-08	1.1E-07				23%	-8.9	-8.8	-10.9
3-mercaptopropionic acid	203-537-0	107-96-0	107960	1473	Reach_723	2030	106	30.2	2.1E+01	7.5E+04	3.3E+00	4.3		3.5E-06	3.5E-07	1.1E-06				14%	-7.8	-8.8	-10.8
619-753-7	264-697-5	64131-85-7	64131857	3426	Reach_2864	2031	477	90.3	2.7E-06	1.1E-01	8.3E+05			3.5E-06	3.5E-08	1.1E-07				14%	-7.9	-8.8	-10.9
N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxo-2-[[2-(triflu	268-734-6	68134-22-5	68134225	3507	Reach_2898	2032	405	251.1	9.8E-11	7.6E+00	1.5E+03	8.65	12.2	1.1E-06	1.1E-07	3.5E-07				14%	-8.2	-8.8	-10.8
2,4'-difluorobenzophenone	263-580-6	62518-65-4	62518654	3374	Reach_2854	2033	204	46.3	4.8E-01	4.0E+00	2.3E+04			3.5E-07	3.5E-08	1.1E-07				15%	-9.1	-8.8	-10.4
trifluoroacetyl chloride	206-556-2	354-32-5	354325	2732	Reach_1245	2034	132	-83.7	3.0E+04	1.9E+05	8.7E-01			1.1E-07	3.5E-08	3.5E-08				19%	-9.2	-8.8	-10.6
(2Z)-but-2-ene-1,4-diyl diacetate	690-722-8	494799-36-9	494799369	2981	Reach_4659	2035	229	163.3	1.9E-05	4.9E+01	1.8E+04			3.5E-06	3.5E-07	1.1E-06				14%	-9.1	-8.8	-10.6
ethyl diphenylphosphinite	201-891-0	89-25-8	89258	3970	Reach_339	2036	174	113.4	4.6E-03	9.5E+04	3.6E+02			1.1E-06	1.1E-07	3.5E-07				15%	-9.1	-8.8	-10.5
616-466-9	265-512-0	65140-91-2	65140912	5971	Reach_2869	2037	695	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				20%	-8.9	-8.8	-10.3
5-methoxy-4-methyl-2,4-dihydro-3H-1,2,4-triazol-3-one	608-385-2	2963-69-1	2963691	2570	Reach_4274	2038	320	195.2	6.9E-10	5.4E+02	2.0E+00	14.8		1.1E-06	3.5E-07	1.1E-06				14%	-7.6	-8.8	-10.9
N,N'-ethane-1,2-diylbis(12-hydroxyoctadecan-1-amide)	204-613-6	123-26-2	123262	1765	Reach_1042	2039	625	349.8	1.6E-22	8.9E-08	2.0E+11	13.8	14.7	1.1E-06	1.1E-07	3.5E-07				15%	-8.0	-8.8	-10.3
2-ethylhexyl laurate	243-697-9	20292-08-4	20292084	2257	Reach_2491	2040	313	81.1	4.2E-03	6.0E-03	4.5E+08			1.1E-06	1.1E-07	3.5E-07				23%	-8.7	-8.8	-10.3
604-075-6	617-892-8	86604-75-3	86604753	6067	Reach_4478	2041	222	0.0												21%	-8.5	-8.8	-10.3
di-tert-butyl peroxide	203-733-6	110-05-4	110054	1514	Reach_803	2042	146	-43.3	3.7E+03	1.8E+02	2.8E+03			1.1E-06	3.5E-07	1.1E-06				20%	-9.1	-8.8	-11.7
2,2'-dithiobis(5-ethoxy-7-fluoro[1,2,4]triazolo[1,5-c]pyrimidine	695-187-4	166524-75-0	166524750	2108	Reach_4689	2043	426	233.2	1.6E-09	2.1E-03	3.0E+03		12.1	3.5E-07	1.1E-07	3.5E-07				16%	-8.5	-8.8	-10.7
3,3,5-trimethylcyclohexan-1-one	212-855-9	873-94-9	873949	3931	Reach_1582	2044	140	6.7	1.2E+02	1.8E+03	2.6E+02			1.1E-06	3.5E-07	1.1E-06				15%	-9.1	-8.8	-10.3
4-hydroxybutyl acrylate	219-606-3	2478-10-6	2478106	1247	Reach_1815	2045	144	6.9	2.3E+00	5.4E+04	5.5E+00	15.6		3.5E-06	3.5E-07	1.1E-06				14%	-8.9	-8.8	-10.9
3,7-dimethylocta-1,6-diene	219-433-3	2436-90-0	2436900	2390	Reach_1809	2046	138	-66.1	6.7E+02	2.5E+00	7.6E+04			1.1E-06	1.1E-07	3.5E-07				21%	-9.1	-8.8	-11.8
α,α,α,2-tetrachlorotoluene	276-017-4	71786-67-9	71786679	6009	Reach_2931	2047	292	0.0												21%	-9.1	-8.8	-10.5
2-methoxy-4-(trifluoromethyl)pyridine-3-sulfonyl chloride	606-871-9	219715-41-0	219715410	2313	Reach_4223	2048	276	109.4	1.6E-02	6.8E+02	1.8E+03			3.5E-07	3.5E-08	1.1E-07				16%	-9.0	-8.9	-10.6
tetramethylene dimethacrylate	218-218-1	2082-81-7	2082817	2277	Reach_1756	2049	226	-46.4	2.5E-02	1.7E+02	1.5E+03			3.5E-06	3.5E-07	1.1E-06				14%	-9.1	-8.9	-10.7
3-methoxy-3-methylbutan-1-ol	231-293-5	7486-38-6	7486386	6022	Reach_2255	2050	190	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-9.1	-8.9	-10.7
1-naphthyl isocyanate	201-703-7	86-84-0	86840	3911	Reach_304	2051	169	41.7	1.3E+00	1.7E+02	5.9E+03			1.1E-06	1.1E-07	3.5E-07				15%	-9.1	-8.9	-10.4
bis(2-ethylhexyl) tetrabromophthalate	247-426-5	26040-51-7	26040517	2450	Reach_2574	2052	706	229.2	2.3E-09	4.8E-07	8.9E+11			1.1E-06	1.1E-07	3.5E-07				24%	-9.1	-8.9	-9.4
(S)-pyrrolidine-2-carboxamide	618-525-4	90315-82-5	90315825	3998	Reach_4496	2053	208	67.4	3.3E-03	2.2E+03	5.9E+01	12.4		1.1E-06	1.1E-07	3.5E-07				14%	-7.9	-8.9	-10.9
(R)-[[(4-ethyl-2,3-dioxopiperazin-1-yl)carbonyl]amino]phenylac	243-248-7	19719-28-9	19719289	2238	Reach_2483	2054	205	97.6	2.3E-02	5.2E+02	5.2E+02	3.98		3.5E-06	3.5E-07	1.1E-06				14%	-7.8	-8.9	-10.8
2-[[(3-amino-4-hydroxyphenyl)sulphonyl]amino]benzoic acid	603-434-4	130755-46-3	130755463	1842	Reach_4120	2055	704	339.7	6.6E-17	6.4E-08	6.8E+06		12.5	3.5E-08	1.1E-08	3.5E-08				14%	-7.8	-8.9	-10.8
potassium 3-sulphonatopropyl acrylate	250-465-0	31098-20-1	31098201	5837	Reach_2652	2056	232	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.5	-8.9	-10.5
N,N''-hexane-1,6-diylbis[N'-benzylurea]	254-274-3	39072-70-3	39072703	2833	Reach_2722	2057	383	249.6	1.2E-10	2.5E+00	6.2E+03	13.4	14	1.1E-06	1.1E-07	3.5E-07				15%	-8.1	-8.9	-10.7
butyl isocyanate	203-862-8	111-36-4	111364	298	Reach_853	2058	99	-39.0	2.6E+03	7.7E+03	1.8E+02			2.4E-07	1.1E-06	3.5E-06				18%	-9.1	-8.9	-10.5
isopropenyl acetate	203-562-7	108-22-5	108225	1478	Reach_735	2059	100	-79.6	5.7E+03	3.7E+04	1.9E+01			3.5E-06	3.5E-07	1.1E-06				14%	-9.1	-8.9	-10.6
1,8-diazabicyclo[5.4.0]undec-7-ene	201-849-1	88-66-4	88664	3962	Reach_328	2060	195	16.3	8.2E+00	1.5E+01	4.2E+03		0	1.1E-07	1.1E-08	3.5E-08				16%	-9.1	-8.9	-10.5
617-343-2	209-947-6	598-72-1	598721	3291	Reach_1405	2061	153	29.7	3.5E+01	1.0E+05	7.1E+00			1.1E-06	3.5E-07	3.5E-07				15%	-9.1	-8.9	-10.5
2-ethoxyethylamine	204-223-6	117-96-4	117964	5277	PharmaUBA	2062	614	284.8	4.8E-13	8.3E-01	2.3E+01			1.1E-06	1.1E-07	3.5E-07				14%	-9.1	-8.9	-10.4
3-(isodecyloxy)propylamine	259-265-8	54634-94-5	54634945	3149	Reach_2801	2063	304	140.2	1.5E-04	2.7E+00	4.2E+05		0	1.1E-06	1.1E-07	3.5E-07				17%	-9.1	-8.9	-10.5
N,N'-(2,5-dimethyl-1,4-phenylene)bis[3-oxobutyramide]	201-321-0	81-07-2	81072	98	Reach_270	2064	183	159.9	1.4E-05	1.3E+03	2.8E+00	1.7	14.4	2.3E-08	3.5E-07	1.1E-06				16%	-7.8	-8.9	-10.7
609-057-1	290-823-3	90268-23-8	90268238	3995	Reach_2991	2065	660	349.8	2.7E-20	1.0E-04	1.3E+07									18%	-8.6	-8.9	-10.5
3,5-dimethylpyridine	209-708-6	591-22-0	591220	3266	Reach_1390	2066	107	-7.6	1.9E+02	2.3E+05	7.9E+01		7.8	3.5E-07	3.5E-08	1.1E-07				16%	-9.0	-8.9	-10.7
manganese, 4-[(4-chloro-5-methyl-2-sulfophenyl)azo]-3-hydro	235-471-3	12238-31-2	12238312	5629	Reach_2310	2067	476	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.5	-8.9	-10.5
3',4',5'-trifluorobiphenyl-2-amine	220-358-3	2736-23-4	2736234	2501	Reach_1860	2068	270	174.9	1.0E-05	3.2E+02	1.6E+01			1.1E-06	1.1E-07	3.5E-07				14%	-8.1	-8.9	-10.9
1,5-dichloro-2-(1-methylethoxy)-4-nitrobenzene	255-259-4	41200-97-9	41200979	2872	Reach_2740	2069	250	101.8	1.9E-02	8.4E+00	1.2E+04			1.1E-06	1.1E-07	3.5E-07				16%	-9.1	-8.9	-10.6
1,1-diphenylethylene	608-371-6	29518-11-4	29518114	2568	Reach_4273	2070	177	102.5	1.1E-02	3.6E+02	3.5E+00			1.1E-06	1.1E-07	3.5E-07				16%	-9.1	-8.9	-10.3
dichloro(phenyl)phosphine	211-425-8	644-97-3	644973	3437	Reach_1480	2071	179	-4.9	1.3E+01	3.1E+02	1.0E+03			3.5E-07	3.5E-08	1.1E-07				17%	-9.1	-8.9	-10.2
nonanoic acid	203-931-2	112-05-0	112050	320	Reach_886	2072	158	59.1	2.9E+00	4.1E+02	3.3E+03	4.9		3.8E-06	3.5E-07	1.1E-06				14%	-8.9	-8.9	-10.8
pyridine-2,3-dicarboxylic acid	605-637-3	172529-93-0	172529930	2128	Reach_4181	2073	328	201.5	2.0E-07	1.3E+02	2.0E+00	12.9		1.1E-06	1.1E-07	3.5E-07				14%	-7.7	-8.9	-10.9
butyric anhydride	203-383-4	106-31-0	106310	1434	Reach_664	2074	158	-44.6	4.8E+01	3.0E+03	2.5E+01			3.5E-06	3.5E-07	1.1E-06				14%	-9.1	-8.9	-10.5
N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-2-[(2-methoxyphe	603-373-3	129909-90-6	129909906	415	Reach_4117	2075	241	176.7	8.0E-06	5.4E+03	1.7E+01	0	12	1.8E-08	1.1E-07	3.5E-07				14%	-8.1	-8.9	-10.9
phthalide	700-156-6	106649-95-0	106649950	5600	Reach_4783	2076	222	0.0												14%	-8.8	-8.9	-10.9
diiodohydroxyquinoline	206-001-4	281-23-2	281232	579	Reach_1220	2077	136	-19.2	3.0E+00	3.5E+00	8.7E+03	0	0	3.7E-09	1.1E-07	3.5E-07				16%	-8.5	-8.9	-10.8

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
bis(2,6-diisopropylphenyl)carbodiimide	218-487-5	2162-74-5	2162745	2300	Reach_1767	2078	363	141.0	1.9E-05	5.8E-04	5.2E+08			3.5E-07	3.5E-08	1.1E-07				23%	-8.8	-8.9	-9.7
618-251-5	244-859-1	22235-81-0	22235810	2323	Reach_2519	2079	317	150.7	6.9E-07	3.9E+03	6.6E+02	14.1	3.93	1.1E-06	1.1E-07	3.5E-07				14%	-7.6	-8.9	-10.8
2-(2-ethoxyethoxy)ethyl acetate	203-940-1	112-15-2	112152	1577	Reach_890	2080	176	1.9	1.9E+01	6.6E+04	2.1E+00			3.5E-06	3.5E-07	1.1E-06				14%	-9.1	-8.9	-10.9
bis(2-(2-butoxyethoxy)ethyl) adipate	205-465-5	141-17-3	141173	1933	Reach_1158	2081	435	117.1	1.1E-04	2.0E+00	1.7E+03			1.1E-06	1.1E-07	3.5E-07				15%	-9.1	-8.9	-10.8
605-446-5	605-446-5	166524-74-9	166524749	2107	Reach_4175	2082	400	222.3	8.4E-09	7.9E-02	3.2E+02		12.5	3.5E-07	3.5E-08	1.1E-07				16%	-8.2	-8.9	-10.8
(3R)-3-aminobutan-1-ol	201-836-0	88-50-6	88506	3958	Reach_325	2083	242	156.7	1.1E-06	3.5E+01	1.6E-01	-1.07	13.5	1.1E-07	1.1E-08	3.5E-08				14%	-9.0	-8.9	-10.9
2,2'-[(2,2',5,5'-tetrachloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N	244-776-0	22094-93-5	22094935	2317	Reach_2516	2084	755	349.8	5.5E-22	4.6E-08	2.5E+09	8.38	13.5	3.5E-09	3.5E-09	3.5E-09				23%	-8.8	-8.9	-9.8
2,3-epoxypropyl o-tolyl ether	218-645-3	2210-79-9	2210799	2319	Reach_1771	2085	164	30.3	5.8E+00	1.5E+03	1.4E+02			3.5E-06	3.5E-07	1.1E-06				14%	-9.1	-8.9	-10.7
(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl 4-(2-hydroxypropan-2-y	241-621-9	17637-11-5	17637115	2146	Reach_2439	2086	490	273.3	9.1E-16	1.5E+03	1.0E-01	0.91	0	1.1E-06	3.5E-07	1.1E-06				16%	-9.1	-8.9	-10.7
5-Amino-2,4-di-tert-butylphenyl methyl carbonate	604-106-3	139007-06-0	139007060	1915	Reach_4141	2087	219	23.8	4.3E-01	3.4E+01	1.5E+05		8.58	1.1E-06	1.1E-07	3.5E-07				16%	-8.5	-8.9	-10.7
(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)(ethoxyimino)acetic acid	619-518-9	18480-53-0	18480530	2193	Reach_4527	2088	198	113.2	1.6E-02	7.9E+02	1.4E+02	3.15	14.6	1.1E-06	1.1E-07	3.5E-07				14%	-8.1	-8.9	-10.8
3,4-dichlorobenzonitrile	229-494-8	6574-99-8	6574998	3456	Reach_2194	2089	172	52.7	1.8E+00	6.3E+01	6.8E+02			1.1E-07	1.1E-08	3.5E-08				19%	-9.2	-8.9	-10.2
thiophene-2-ethylamine	230-947-7	7379-51-3	7379513	3626	Reach_2243	2090	168	71.4	1.1E-01	1.3E+03	1.6E+03			1.1E-06	1.1E-07	3.5E-07				14%	-9.1	-8.9	-10.4
1H-imidazole-1-propylamine	272-701-1	68909-32-0	68909320	3530	Reach_2912	2091	297	128.0	2.2E-04	8.8E-02	2.2E+05		9.19	1.1E-06	1.1E-07	3.5E-07				14%	-7.9	-8.9	-11.0
Ethyl 4-(2-hydroxypropan-2-yl)-2-propyl-1H-imidazole- 5-carbo	619-880-8	176972-62-6	176972626	2151	Reach_4552	2092	258	115.5	4.4E-05	6.3E+02	6.0E+01	10.3		1.1E-06	1.1E-07	3.5E-07				14%	-8.0	-8.9	-10.9
ethyl 4-hydroxybenzoate	204-399-4	120-47-8	120478	14	Reach_995	2093	166	61.8	1.2E-02	1.6E+03	3.1E+02	8.5		6.3E-07	3.5E-07	1.1E-06				15%	-8.7	-8.9	-10.7
octabenzone	217-421-2	1843-05-6	1843056	2191	Reach_1725	2094	326	177.3	9.2E-06	2.3E-01	9.1E+06	9.73		1.1E-06	1.1E-07	3.5E-07				21%	-8.5	-8.9	-10.1
(4aR,7S,8aR)-9,9-dimethyltetrahydro-4a,7-methanooxazireno[3	202-384-7	95-02-3	95023	4117	Reach_421	2095	138	100.9	1.0E-01	1.0E+06	1.9E-02			3.5E-07	1.1E-07	3.5E-07				16%	-8.4	-8.9	-10.7
605-999-2	250-099-1	30246-33-4	30246334	2589	Reach_2644	2096	344	323.2	2.1E-12	8.0E+01	1.2E-01	2.19		3.5E-07	1.1E-07	3.5E-07				14%	-8.0	-8.9	-10.9
(2-hydroxy-3-sulphopropyl)dimethyl[3-[(1-oxododecyl)amino]p	242-893-1	19223-55-3	19223553	5755	Reach_2475	2097	441	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.6	-8.9	-10.6
2,2,4(or 2,4,4)-trimethylhexanedinitrile	800-052-1	1421439-99-7	1421439997	5693	Reach_5036	2098	744	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				16%	-9.0	-8.9	-10.7
4,4'-methylenebis(2,6-xylidine)	244-912-9	22326-31-4	22326314	2329	Reach_2522	2099	246	205.9	8.3E-10	3.3E+04	4.0E-02		0	3.5E-06	3.5E-07	1.1E-06				16%	-8.5	-8.9	-10.7
methyl 3-{1,4-dioxaspiro[4.5]dec-8-yl[(trans-4-methylcyclohex	219-281-8	2402-77-9	2402779	2366	Reach_1795	2100	148	18.7	4.0E+01	1.1E+03	1.2E+02			1.1E-07	1.1E-08	3.5E-08				20%	-8.4	-8.9	-10.3
decan-4-olide	211-892-8	706-14-9	706149	813	Reach_1518	2101	170	20.2	6.8E-01	2.0E+02	3.7E+02			4.8E-07	3.5E-08	1.1E-07				16%	-9.1	-8.9	-10.5
606-548-2	611-869-6	59721-67-4	59721674	3285	Reach_4366	2102	216	76.5	3.5E-02	8.4E-01	9.5E+04			1.1E-06	1.1E-07	3.5E-07				14%	-8.0	-8.9	-10.9
3α,7α-dihydroxy-12-oxo-5β-cholan-24-oic acid	218-561-7	2182-55-0	2182550	2306	Reach_1769	2103	126	-45.2	6.3E+02	1.2E+03	4.9E+02	0		1.1E-06	3.5E-07	1.1E-06				14%	-8.2	-8.9	-10.8
3-(1-cyanoethyl)benzoyl chloride	219-535-8	2457-01-4	2457014	5578	Reach_1812	2104	424	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				16%	-9.1	-8.9	-10.7
cis-hex-3-en-1-ol	213-192-8	928-96-1	928961	1016	Reach_1602	2105	100	-38.5	1.2E+02	2.7E+04	4.1E+01	15.9		4.6E-07	1.1E-06	3.5E-06				16%	-9.2	-8.9	-10.4
2,2,4-trimethylpentane	208-759-1	540-84-1	540841	3122	Reach_1335	2106	114	-86.0	5.9E+03	2.0E+00	1.2E+04			1.1E-06	3.5E-07	1.1E-06				21%	-9.2	-8.9	-11.9
8-chlorotheophylline	201-590-4	85-18-7	85187	3883	Reach_292	2107	215	202.0	1.5E-08	2.1E+04	1.8E+00	4.85		3.5E-07	3.5E-08	1.1E-07				16%	-7.8	-8.9	-10.8
α-ethyl-p-methoxybenzyl alcohol	226-315-5	5349-60-0	5349600	3104	Reach_2101	2108	166	37.9	1.5E-01	4.4E+03	1.2E+02	15.2		1.1E-06	1.1E-07	3.5E-07				14%	-8.9	-8.9	-10.8
3,4-dichlorophenyl isocyanate	211-790-3	696-23-1	696231	3545	Reach_1511	2109	127	106.6	1.8E-04	4.4E+03	2.6E+00			1.1E-06	3.5E-08	1.1E-07				20%	-9.2	-8.9	-10.3
(E)-3-formylbut-2-enyl acetate	247-825-4	26586-02-7	26586027	2480	Reach_2589	2110	142	-17.4	4.3E+01	3.8E+04	4.9E+00			3.5E-06	3.5E-07	1.1E-06				14%	-9.1	-8.9	-10.8
3-(triethoxysilyl)propanethiol	279-914-9	82199-12-0	82199120	3820	Reach_2963	2111	367	260.6	2.2E-11	9.5E+01	1.9E+02	8.73		1.1E-06	1.1E-07	3.5E-07				16%	-9.2	-8.9	-10.5
hexamethylcyclotrisiloxane	208-765-4	541-05-9	541059	3126	Reach_1339	2112	222	1.1	4.4E+02	3.4E+01	4.4E+05			3.5E-09	3.5E-09	3.5E-09				24%	-9.3	-8.9	-11.5
malic acid	230-022-8	6915-15-7	6915157	3533	Reach_2210	2113	134	112.7	3.9E-04	3.4E+05	2.1E-02	3.63		3.5E-06	3.5E-07	1.1E-06				14%	-7.6	-8.9	-10.9
2,2-dimethylpropane-1,3-diyl cyclohex-4-ene-1,2-dicarboxylate	255-180-5	41026-17-9	41026179	2868	Reach_2733	2114	408	219.1	1.1E-08	5.7E+02	4.5E+03	4.09		1.1E-06	1.1E-07	3.5E-07				14%	-8.3	-8.9	-10.9
3,6,9-trioxaundecane-1,11-diol	203-989-9	112-60-7	112607	1594	Reach_915	2115	194	82.9	1.5E-03	1.7E+07	9.5E-03	14.6		1.1E-06	3.5E-07	1.1E-06				14%	-7.8	-8.9	-11.0
2,2,6,6-tetramethyl-4-oxopiperidinooxy	220-778-7	2896-70-0	2896700	2550	Reach_1881	2116	171	103.6	4.9E-04	5.3E+04	1.1E+00		10.1	1.1E-06	3.5E-07	1.1E-06				14%	-7.9	-8.9	-10.9
pentan-1-ol	246-349-4	24605-36-5	24605365	5791	Reach_2550	2117	297	0.0												14%	-9.1	-8.9	-10.6
N,N'-bis(3-aminopropyl)ethylenediamine	234-147-9	10563-26-5	10563265	1417	Reach_2297	2118	174	87.9	9.2E-02	1.0E+06	2.2E-02		3.46	1.1E-05	3.5E-07	1.1E-06				14%	-7.9	-8.9	-11.1
methyl 4-acetamido-5-iodo-2-methoxybenzoate	607-206-5	23175-18-0	23175180	2346	Reach_4235	2119	271	152.9	1.7E-07	3.2E+03	4.2E+01	14.2		1.1E-06	1.1E-07	3.5E-07				16%	-8.2	-8.9	-10.7
N,N'-(methylenedi-p-phenylene)bis[hexahydro-2-oxo-1H-azepi	258-981-8	54112-23-1	54112231	3127	Reach_2797	2120	477	349.8	8.8E-18	1.1E+00	3.0E+04	14	13.6	1.1E-06	3.5E-08	1.1E-07				16%	-8.1	-8.9	-10.7
N,N-dimethylacrylamide	220-237-5	2680-03-7	2680037	1254	Reach_1852	2121	99	-17.7	3.6E+02	6.8E+05	7.4E-01		14.4	3.5E-06	3.5E-07	1.1E-06				14%	-9.1	-8.9	-10.9
5-chloro-2-nitrophenol	700-556-0	66682-07-3	66682073	3478	Reach_4933	2122	299	77.3	1.4E-01	8.7E-02	6.8E+05			1.1E-07	1.1E-08	3.5E-08				14%	-8.8	-8.9	-10.9
hydroxycyclohexyl phenyl ketone	213-426-9	947-19-3	947193	4112	Reach_1616	2123	204	93.5	9.4E-04	4.9E+01	2.8E+02	13.4		3.5E-06	3.5E-07	1.1E-06				14%	-8.8	-8.9	-10.8
619-293-7	700-069-3	265136-65-0	265136650	2473	Reach_4750	2124	318	223.1	7.5E-09	2.2E+03	4.2E+00			1.1E-06	1.1E-07	3.5E-07				14%	-8.0	-8.9	-10.9
1-(2-hydroxyethyl)imidazolidin-2-one	208-807-1	542-28-9	542289	3136	Reach_1347	2125	100	-31.7	1.8E+01	3.4E+04	1.5E+00			3.5E-06	3.5E-07	1.1E-06				14%	-7.9	-8.9	-11.0
dibutyl hydrogen phosphate	203-509-8	107-66-4	107664	1467	Reach_713	2126	210	59.3	5.1E-03	1.6E+06	1.9E+02	1.5		1.1E-06	1.1E-07	3.5E-07				14%	-8.2	-8.9	-10.9
4,4'-dinitrostilbene-2,2'-disulphonic acid	204-885-6	128-42-7	128427	1821	Reach_1110	2127	430	295.4	1.3E-17	6.2E+02	1.1E+00	-0.55		1.1E-06	3.5E-08	1.1E-07				14%	-7.7	-8.9	-11.1
2,2,4(or 2,4,4)-trimethyladipic acid	255-679-8	42142-52-9	42142529	2890	Reach_2750	2128	165	50.9	4.8E-02	9.0E+03	9.5E+00	14.3		1.1E-06	1.1E-07	3.5E-07				14%	-8.1	-8.9	-10.9
601-722-4	601-722-4	120570-77-6	120570776	1716	Reach_4102	2129	162	-60.1	2.0E+02	1.2E+06	1.1E-01			3.5E-06	3.5E-07	1.1E-06				14%	-9.1	-8.9	-11.0
2-aminopropane-1,3-diol	208-584-0	534-03-2	534032	3100	Reach_1331	2130	91	26.4	2.2E+00	5.6E+05	2.8E-02	14.4	5.2	3.5E-06	1.1E-06	3.5E-06				14%	-8.2	-8.9	-11.0
cyclohexylurea	211-822-6	698-90-8	698908	3551	Reach_1514	2131	142	70.9	3.1E-01	2.0E+04	1.5E+01	14.3	13.9	1.1E-06	3.5E-07	1.1E-06				14%	-8.8	-8.9	-10.8
methyl formylphenylacetate	201-975-7	90-20-0	90200	3993	Reach_361	2132	319	260.8	9.9E-15	6.5E+04	4.7E-03	-0.78		1.1E-06	1.1E-07	1.1E-06				14%	-8.7	-8.9	-10.9
2,2',6,6'-tetra-tert-butyl-4,4'-methylenediphenol	204-279-1	118-82-1	118821	1679	Reach_971	2133	425	208.5	1.6E-09	5.4E-05	9.8E+08	11		3.5E-06	3.5E-07	1.1E-06				23%	-8.6	-8.9	-9.6
Methyl 3-amino-4-methylbenzoate	207-692-5	488-98-2	488982	2978	Reach_1294	2134	213	15.6	4.5E+01	3.2E+01	1.3E+04			3.5E-07	3.5E-08	1.1E-07				14%	-8.2	-8.9	-10.9
m-(1-cyanoethyl)benzoic acid	700-389-3	20208-39-3	20208393	2254	Reach_4884	2135	276	63.3	1.4E-01	1.4E+02	4.8E+01			3.5E-06	3.5E-07	1.1E-06				14%	-8.2	-8.9	-10.9
3-chloropropionic acid	203-534-4	107-94-8	107948	1471	Reach_721	2136	109	22.4	2.6E+02	1.2E+05	6.8E+00	4		3.5E-06	3.5E-07	1.1E-06				14%	-8.0	-8.9	-10.9
1-(N,N-bis(2-hydroxyethyl)amino)propan-2-ol	229-764-5	6712-98-7	6712987	3486	Reach_2204	2137	163	81.8	7.0E-04	8.1E+05	8.7E-03	14.5	6.2	3.5E-06	1.1E-06	3.5E-06				14%	-7.9	-8.9	-11.0
ethyl 2-cyano-3-ethoxyacrylate	202-624-0	97-97-2	97972	4176	Reach_492	2138	125	-60.3	1.5E+03	1.8E+04	3.0E+00			3.5E-07	1.1E-07	3.5E-07				14%	-9.1	-8.9	-10.9
2,2'-isopropylidenebis(p-phenyleneoxy)diethanol	605-955-2	181997-72-8	181997728	2174	Reach_4186	2139	247	126.6	1.2E-03	2.9E+02	2.8E+01	0		1.1E-06	1.1E-07	3.5E-07				16%	-8.2	-8.9	-10.7
tributylamine	203-058-7	102-82-9	102829	156	Reach_600	2140	185	0.8	2.1E+01	3.3E+01	2.9E+04		3	9.8E-09	3.5E-08	1.1E-07				23%	-9.2	-8.9	-10.8
2-tert-butylhydroquinone	217-752-2	1948-33-0	1948330	523	Reach_1737	2141	166	83.3	1.7E-02	1.0E+03	8.7E+02	10.1		1.7E-08	1.1E-06	3.5E-06				22%	-9.0	-8.9	-10.1
609-262-6	609-262-6	36589-61-4	36589614	5860	Reach_4295	2142	240	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.6	-8.9	-10.6
Diammonium 5-(hexylsulfonyl)-2-{[3-methyl-2,7-dioxo-1-(3-sul	700-712-8	1054448-65-5	1054448655	5595	Reach_4975	2143	799	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.6	-8.9	-10.6
tetrabromophthalic anhydride	211-185-4	632-79-1	632791	3396	Reach_1473	2144	464	152.9	2.7E-06	2.1E-01	4.3E+05			1.1E-06	1.1E-07	3.5E-07				19%	-8.7	-8.9	-10.6
warfarin	216-731-5	1655-07-8	1655078	2100	Reach_1705	2145	170	34.8	2.6E+00	6.5E+03	1.2E+01	13		3.5E-06	3.5E-07	1.1E-06				16%	-8.2	-8.9	-10.8
propyloxirane	213-701-3	1003-14-1	1003141	1299	Reach_1633	2146	86	-74.0	1.2E+04	1.9E+04	2.2E+01			1.1E-06	1.1E-07	3.5E-07				15%	-9.2	-8.9	-10.8
(3-chloropropyl)dimethoxymethylsilane	242-056-0	18171-19-2	18171192	2172	Reach_2455	2147	183	-21.0	1.3E+02	5.6E+02	6.6E+01			1.1E-07	3.5E-08	1.1E-07				20%	-9.2	-8.9	-10.7
6,6'-di-tert-butyl-4,4'-butylidenedi-m-cresol	201-618-5	85-60-9	85609	3893	Reach_298	2148	383	199.8	7.0E-09	9.4E-04	1.2E+09	10.5		1.1E-06	1.1E-07	3.5E-07				23%	-8.7	-8.9	-9.5
lauroyl chloride	203-941-7	112-16-3	112163	1578	Reach_891	2149	219	37.3	2.3E+00	2.7E-01	2.8E+04			3.5E-07	3.5E-08	1.1E-07				22%	-9.2	-8.9	-11.5
1,2-dimethoxyethane	203-794-9	110-71-4	110714	1528	Reach_825	2150	90	-82.3	1.1E+04	3.4E+05	6.2E-01			1.1E-06	1.1E-07	3.5E-07				14%	-9.2	-8.9	-10.4
600-593-1	700-509-4	19294-29-2	19294292	5756	Reach_4915	2151	194	0.0												14%	-8.1	-8.9	-10.9
1,2-dimethylimidazole	700-555-5	1233733-31-7	1233733317	5633	Reach_4932	2152	1120	0.0	0.0E+00	0.0E+00	0.0E+00		0	0.0E+00	0.0E+00	0.0E+00				16%	-9.2	-8.9	-10.7

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
thiodiethylene bis[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propior	255-392-8	41484-35-9	41484359	2878	Reach_2743	2153	643	289.4	1.0E-15	3.9E-07	2.3E+10	11.6		1.1E-06	1.1E-07	3.5E-07				24%	-9.0	-8.9	-9.5
2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol	248-908-8	28219-61-6	28219616	2525	Reach_2615	2154	208	60.2	9.6E-03	1.4E+01	1.4E+05	15.5		1.1E-06	3.5E-07	1.1E-06				18%	-9.0	-8.9	-10.6
methylhydrazine	200-471-4	60-34-4	60344	752	Reach_58	2155	46	-57.6	8.5E+03	6.7E+05	1.0E-01		6	4.5E-06	1.1E-07	3.5E-07				14%	-9.2	-8.9	-10.8
3-methoxybutan-1-ol	219-741-8	2517-43-3	2517433	2422	Reach_1827	2156	104	-43.5	1.2E+02	5.3E+04	1.0E+00	15.5		3.5E-06	3.5E-07	1.1E-06				14%	-9.2	-8.9	-10.8
cytosine	800-303-5	1083057-14-0	1083057140	1482	Reach_5043	2157	284	149.1	7.1E-05	1.0E+01	2.2E+04		8.06	1.1E-06	1.1E-07	3.5E-07				14%	-7.9	-8.9	-10.9
(3,4-diethoxyphenyl)acetonitrile	218-849-2	2253-52-3	2253523	2335	Reach_1780	2158	242	-38.6	6.4E-01	1.6E+01	1.1E+04			1.1E-06	1.1E-07	1.1E-06				16%	-9.2	-8.9	-10.7
methacrylonitrile	204-817-5	126-98-7	126987	1809	Reach_1093	2159	67	-68.7	7.5E+03	9.3E+04	5.8E+00			3.5E-07	1.1E-07	3.5E-07				16%	-9.2	-8.9	-10.2
603-436-5	214-230-6	1115-70-4	1115704	5607	Reach_1649	2160	166	0.0												14%	-8.0	-8.9	-10.9
dimethyl glutarate	214-277-2	1119-40-0	1119400	1564	Reach_1654	2161	160	-83.3	2.4E+01	1.2E+04	7.9E+00			3.5E-06	3.5E-07	1.1E-06				14%	-9.2	-8.9	-10.8
meglumine	203-977-3	112-49-2	112492	330	Reach_909	2162	178	2.0	3.2E+01	2.8E+05	1.7E-01	0	0	9.2E-07	1.1E-07	1.1E-06				16%	-8.0	-8.9	-10.8
(Z)-cyclooctene	201-944-8	89-83-8	89838	996	Reach_353	2163	150	38.1	2.2E+00	5.6E+02	3.3E+03			2.6E-08	3.5E-07	1.1E-06				22%	-9.2	-8.9	-11.7
2,4-dichlorophenylacetic acid	613-982-6	66742-57-2	66742572	3482	Reach_4393	2164	230	98.7	9.0E-03	2.0E+01	5.0E+03			1.1E-06	1.1E-07	3.5E-07				14%	-8.3	-8.9	-10.9
tris(oxiranylmethyl) benzene-1,2,4-tricarboxylate	230-638-7	7237-83-4	7237834	3604	Reach_2233	2165	378	161.7	5.2E-06	1.3E+03	1.3E+00			1.1E-06	1.1E-07	3.5E-07				14%	-7.9	-9.0	-11.1
N-[4-(aminocarbonyl)phenyl]-4-[[1-[[(2,3-dihydro-2-oxo-1H-be	202-485-6	96-17-3	96173	1046	Reach_452	2166	86	-79.3	1.4E+03	2.0E+04	1.7E+01	0	0	7.4E-07	1.1E-06	3.5E-06				14%	-8.1	-9.0	-10.9
5-ethyl-1,3-dioxane-5-methanol	225-967-8	5187-23-5	5187235	3048	Reach_2083	2167	146	30.3	1.4E+00	4.3E+03	1.2E+00	15.1		1.1E-06	3.5E-07	1.1E-06				14%	-9.2	-9.0	-10.9
propylamine	203-462-3	107-10-8	107108	208	Reach_693	2168	59	-71.7	4.1E+04	1.0E+06	2.2E+00		4	4.1E-07	1.1E-06	3.5E-06				16%	-9.2	-9.0	-10.2
Cuprate(4-), [2-[[[[2-hydroxy-3-sulfo-5-[[2-(sulfooxy)ethyl]sulfo	291-103-1	90341-71-2	90341712	6079	Reach_2993	2169	858	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.6	-9.0	-10.6
dimethyl propylphosphonate	242-555-3	18755-43-6	18755436	2206	Reach_2468	2170	152	-24.7	6.5E+01	1.6E+04	2.5E+00			1.1E-06	1.1E-07	1.1E-06				14%	-9.2	-9.0	-10.6
2,4,6,8-tetramethylcyclotetrasiloxane	219-137-4	2370-88-9	2370889	2355	Reach_1786	2171	236	-42.9	1.1E+03	4.1E+03	4.0E+04			3.5E-09	3.5E-09	3.5E-09				24%	-9.3	-9.0	-10.9
2,6-di-tert-butyl-4-(4,6-bis(octylthio)-1,3,5-triazin-2-ylamino)ph	213-590-1	991-84-4	991844	4197	Reach_1625	2172	589	289.8	1.2E-14	5.7E-09	1.8E+13	10.3	10.8	1.1E-06	1.1E-07	3.5E-07				21%	-9.2	-9.0	-9.5
p-isopropylphenyl isocyanate	229-959-5	6860-97-5	6860975	3521	Reach_2209	2173	474	334.2	6.5E-21	1.2E-01	5.9E-01			1.1E-06	3.5E-08	3.5E-07				17%	-9.2	-9.0	-10.2
diethyl [2-(2,4-difluorophenyl)prop-2-en-1-yl]malonate	200-090-3	51-34-3	51343	3036	Reach_15	2174	303	151.3	2.6E-07	7.5E+03	2.5E+00	14.1		1.1E-06	1.1E-07	3.5E-07				16%	-9.2	-9.0	-10.5
allantoin	202-592-8	97-59-6	97596	4166	Reach_481	2175	158	194.4	1.7E-07	1.3E+03	7.2E-04	9	14.8	3.5E-06	3.5E-07	1.1E-06				14%	-7.7	-9.0	-11.0
4-chlorophthalic anhydride	211-754-7	693-57-2	693572	3540	Reach_1508	2176	215	305.7	4.3E-09	5.7E+00	2.1E+00			1.1E-06	1.1E-07	3.5E-07				15%	-9.2	-9.0	-10.6
Androsta-4,9(11)-diene-3,17-dione	616-391-1	76812-02-7	76812027	3725	Reach_4438	2177	542	273.7	3.8E-15	7.7E-03	2.6E+07			1.1E-06	1.1E-07	3.5E-07				16%	-9.0	-9.0	-10.8
620-037-1	617-458-8	83393-23-1	83393231	6048	Reach_4464	2178	252	0.0												14%	-9.2	-9.0	-10.5
(S)-(+)-1-methoxy-2-propylamine	617-448-3	83196-56-9	83196569	3842	Reach_4462	2179	311	184.8	3.3E-08	2.1E+02	7.4E+02			3.5E-07	1.1E-07	3.5E-07				14%	-9.2	-9.0	-10.5
succinimide	204-635-6	123-56-8	123568	1771	Reach_1053	2180	99	148.9	4.8E-02	2.2E+05	1.4E-01	9.3		3.5E-06	3.5E-07	1.1E-06				14%	-8.0	-9.0	-11.1
dicyclohexyl phthalate	201-545-9	84-61-7	84617	3871	Reach_286	2181	330	61.5	6.1E-04	1.6E+02	1.6E+06			1.1E-06	1.1E-07	3.5E-07				20%	-8.6	-9.0	-10.4
2-(2-chloroethoxy)ethanol	211-059-9	628-89-7	628897	3380	Reach_1461	2182	125	-12.6	1.3E+01	5.2E+05	6.9E-01	14.9		3.5E-07	1.1E-07	3.5E-07				16%	-8.9	-9.0	-10.9
2-ethylhexylamine	203-233-8	104-75-6	104756	169	Reach_628	2183	129	-21.0	2.2E+02	3.6E+02	5.4E+02		4	2.2E-07	3.5E-08	1.1E-07				19%	-9.3	-9.0	-10.8
methyl 4-hydroxybenzoate	202-785-7	99-76-3	99763	4216	Reach_538	2184	152	51.5	1.1E-01	5.6E+03	1.0E+02	8.5		1.1E-05	1.1E-06	3.5E-06				14%	-8.9	-9.0	-10.8
4-bromo-1,2-dichlorobenzene	607-674-0	25260-60-0	25260600	2425	Reach_4247	2185	172	-72.3	6.7E+01	1.2E+04	1.5E+01			3.5E-06	3.5E-07	1.1E-06				22%	-9.3	-9.0	-10.9
[3R-(3α,3aβ,7β,8aα)]-1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetram	202-377-9	94-96-2	94962	1024	Reach_420	2186	146	13.2	4.0E-01	1.0E+04	4.0E+01			4.6E-07	3.5E-07	1.1E-06				18%	-9.2	-9.0	-10.6
L-proline	205-702-2	147-85-3	147853	1999	Reach_1197	2187	115	294.4	6.2E-06	2.8E+05	7.1E-03	1.9	3.4	3.5E-06	3.5E-07	1.1E-06				14%	-7.7	-9.0	-11.0
603-266-1	212-079-0	760-23-6	760236	870	Reach_1530	2188	125	-68.6	2.5E+03	4.4E+03	4.0E+02	0		2.5E-08	1.1E-08	3.5E-08				16%	-8.3	-9.0	-10.7
methyl chloroacetate	202-501-1	96-34-4	96344	4145	Reach_463	2189	109	-61.0	1.4E+03	5.8E+04	4.3E+00			3.5E-06	3.5E-07	1.1E-06				14%	-9.2	-9.0	-10.6
2-(diethylamino)-6-methyl-1H-pyrimidin-4-one	206-278-1	320-60-5	320605	2642	Reach_1234	2190	215	1.5	1.5E+02	8.3E+00	1.7E+04			1.1E-07	1.1E-08	3.5E-08				14%	-8.1	-9.0	-10.9
Disodium 4-amino-5-hydroxy-3,6-bis{(E)-[4-(vinylsulfonyl)phen	695-988-9	100556-82-9	100556829	5591	Reach_4699	2191	752	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.7	-9.0	-10.6
δ-valerolactone	236-143-2	13188-60-8	13188608	5664	Reach_2326	2192	347	0.0												14%	-9.2	-9.0	-10.9
octanal	225-625-8	4979-32-2	4979322	2990	Reach_2069	2193	347	192.3	8.2E+00	3.4E-02	8.9E+05			3.5E-07	3.5E-08	1.1E-07				16%	-9.3	-9.0	-10.8
hexanoic acid	205-550-7	142-62-1	142621	462	Reach_1179	2194	116	26.2	3.7E+01	1.2E+04	1.1E+02	4.9		4.0E-06	3.5E-07	1.1E-06				14%	-8.8	-9.0	-10.9
triethoxy(2,4,4-trimethylpentyl)silane	252-558-1	35435-21-3	35435213	2734	Reach_2690	2195	276	39.8	9.9E-01	8.3E+00	1.1E+04			3.5E-07	1.1E-07	3.5E-07				18%	-9.3	-9.0	-10.6
di(tert-butyl) carbonate	246-240-1	24424-99-5	24424995	2393	Reach_2545	2196	218	-13.0	3.8E+00	1.9E+02	7.4E+01			1.1E-06	1.1E-07	3.5E-07				15%	-9.2	-9.0	-10.5
1-(2,4-dichlorophenyl)ethan-1-one	218-780-8	2234-16-4	2234164	541	Reach_1776	2197	189	50.4	2.9E+00	4.9E+01	9.1E+02			8.5E-08	1.1E-08	3.5E-08				20%	-9.3	-9.0	-10.4
(E)-anethole	224-052-0	4180-23-8	4180238	635	Reach_2019	2198	148	-0.7	8.5E+00	1.4E+02	2.5E+03			1.1E-07	1.1E-07	3.5E-07				19%	-9.3	-9.0	-10.3
1,3-bis(isocyanatomethyl)benzene	222-852-4	3634-83-1	3634831	2766	Reach_1978	2199	188	81.9	1.2E-01	3.5E+03	1.0E+03			3.5E-06	3.5E-07	1.1E-06				14%	-9.1	-9.0	-10.9
2-methylpropane-2-thiol	200-890-2	75-66-1	75661	3679	Reach_157	2200	90	-82.3	2.2E+04	4.4E+03	1.4E+02	11.3		1.1E-06	3.5E-07	1.1E-06				18%	-9.3	-9.0	-11.5
N-[3-(dimethylamino)propyl]stearamide	231-609-1	7651-02-7	7651027	1289	Reach_2266	2201	369	196.2	2.2E-07	5.8E-04	2.2E+07	14.8	4.8	1.1E-06	1.1E-07	3.5E-07				21%	-8.6	-9.0	-10.1
2,4-dichlorophenyl isocyanate	200-749-5	71-30-7	71307	3580	Reach_100	2202	111	91.1	2.8E-04	9.6E+03	3.4E-02			3.5E-06	1.1E-06	3.5E-06				20%	-9.3	-9.0	-10.5
dioctadecyl ether	228-567-1	6297-03-6	6297036	1281	Reach_2163	2203	523	212.9	1.9E-08	8.0E-11	5.8E+16			1.1E-06	1.1E-07	3.5E-07				24%	-9.2	-9.0	-7.6
3,7-dimethyloctan-3-ol	201-133-9	78-69-3	78693	3755	Reach_204	2204	158	-11.8	9.5E+00	4.6E+01	4.0E+03	16		1.1E-06	1.1E-07	3.5E-07				16%	-9.3	-9.0	-10.6
tripropylamine	203-047-7	102-69-2	102692	154	Reach_595	2205	143	-33.7	4.0E+02	1.6E+03	9.8E+02		3	7.1E-08	3.5E-08	3.5E-07				21%	-9.3	-9.0	-10.7
N-(2,6-difluorophenyl)-5-methyl[1,2,4]triazolo[1,5-a]pyrimidine	619-383-6	98967-40-9	98967409	1081	Reach_4516	2206	325	190.0	2.0E-07	2.9E+02	3.2E+01	5.02	12	3.7E-09	1.1E-07	3.5E-07				23%	-8.5	-9.0	-10.0
602-965-9	615-927-1	7319-16-6	7319166	3614	Reach_4419	2207	72	-101.4	3.4E+04	2.1E+04	6.8E+00	0		1.1E-06	3.5E-07	1.1E-06				17%	-9.2	-9.0	-10.8
2-ethyl-2-[[(1-oxoheptyl)oxy]methyl]propane-1,3-diyl bisheptar	203-904-5	111-75-1	111751	1556	Reach_868	2208	117	-0.2	1.0E+01	4.2E+05	2.1E+00			3.5E-06	1.1E-06	3.5E-06				23%	-8.8	-9.0	-9.6
4-bromophenyl acetate	217-668-6	1927-95-3	1927953	2229	Reach_1735	2209	215	38.9	3.3E+00	6.4E+01	3.0E+02			3.5E-07	3.5E-08	3.5E-07				17%	-9.3	-9.0	-10.4
di-sec-butylphenol, mixed isomers	226-854-6	5510-99-6	5510996	3160	Reach_2120	2210	206	76.3	9.8E-01	5.4E+01	3.6E+04	11.3		1.1E-06	1.1E-07	3.5E-07				17%	-9.2	-9.0	-10.5
2,2'-ethylenedioxydiethyl dimethacrylate	203-652-6	109-16-0	109160	1495	Reach_772	2211	286	5.8	1.3E-01	4.0E+02	4.6E+01			3.5E-06	3.5E-07	1.1E-06				14%	-9.2	-9.0	-11.0
602-890-1	602-890-1	122731-58-2	122731582	1757	Reach_4106	2212	284	232.9	1.9E-12	1.5E+04	1.9E-01	3.11		3.5E-06	1.1E-07	3.5E-07				14%	-7.7	-9.0	-11.2
687-796-9	235-557-0	12286-65-6	12286656	5631	Reach_2311	2213	851	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.7	-9.0	-10.7
calcium bis[3-nitro-4-[[2-oxo-1-[(phenylamino)carbonyl]propyl	200-795-6	73-22-3	73223	3616	Reach_106	2214	204	279.0	2.6E-07	5.2E+03	6.0E-02									18%	-8.7	-9.0	-10.7
(E,E,E)-2,7-dimethylocta-2,4,6-trienedial	611-255-8	55314-16-4	55314164	3166	Reach_4354	2215	176	66.7	3.7E-01	7.8E+04	9.3E-01			3.5E-07	3.5E-08	1.1E-07				14%	-9.2	-9.0	-10.9
1-chlorooctane	203-915-5	111-85-3	111853	1561	Reach_876	2216	149	-36.3	1.2E+02	2.5E+00	3.3E+04			1.1E-06	1.1E-07	3.5E-07				21%	-9.3	-9.0	-11.9
4-[[(2-aminophenyl)methyl]amino]cyclohexyl acetate	616-785-3	80012-43-7	80012437	3785	Reach_4444	2217	249	160.4	8.7E-05	3.7E+02	3.5E+02		5	1.1E-06	1.1E-07	3.5E-07				14%	-8.3	-9.0	-10.9
2,6-dichloro-N-(2,6-dimethylphenyl)hexanamide	200-385-7	58-55-9	58559	730	Reach_47	2218	180	193.3	7.4E-08	9.3E+04	4.1E-01	8.7	0	7.0E-09	1.1E-07	3.5E-07				16%	-8.6	-9.0	-10.9
1,3,5-triisopropyl-2,4-dinitrobenzene	247-578-2	26272-90-2	26272902	2460	Reach_2578	2219	305	83.6	7.1E-03	5.7E-04	3.2E+07			1.1E-06	1.1E-07	3.5E-07				19%	-9.2	-9.0	-10.5
619-511-0	244-104-6	20893-30-5	20893305	2280	Reach_2501	2220	123	40.8	4.5E+00	8.1E+02	2.4E+01			1.1E-06	3.5E-08	1.1E-07				19%	-9.3	-9.0	-10.4
2,6-dichlorotoluene	204-269-7	118-69-4	118694	1676	Reach_968	2221	161	3.6	4.8E+01	6.1E+01	6.8E+03			1.1E-07	1.1E-08	3.5E-08				21%	-9.3	-9.0	-10.9
5-methylhexan-2-one	203-737-8	110-12-3	110123	273	Reach_804	2222	114	-54.3	8.9E+02	4.0E+03	4.6E+01			5.3E-07	3.5E-07	1.1E-06				16%	-9.3	-9.0	-10.6
2-methylbut-2-ene	208-156-3	513-35-9	513359	3033	Reach_1317	2223	70	-116.2	6.2E+04	3.1E+02	4.4E+02			1.1E-06	3.5E-07	1.1E-06				20%	-9.3	-9.0	-12.0
(2,4,6-trioxotriazine-1,3,5(2H,4H,6H)-triyl)tris(hexamethylene)	204-642-4	123-68-2	123682	1773	Reach_1055	2224	156	-22.3	9.6E+01	5.0E+02	1.5E+03		0	3.5E-06	3.5E-07	1.1E-06				23%	-8.9	-9.0	-9.6
2,3-didehydro-D-erythro-hexono-1,4-lactone	201-928-0	89-65-6	89656	3982	Reach_349	2225	176	155.7	2.4E-08	2.0E+05	1.3E-02	4.2		3.5E-06	3.5E-07	1.1E-06				14%	-7.7	-9.0	-11.1
pentapotassium ({[(hydroxyphosphinato)methyl](phosphonatc	700-903-6	255830-15-0	255830150	2438	Reach_5021	2226	128	-25.1	4.1E+03		2.8E+00			1.1E-06	3.5E-07	1.1E-06				14%	-9.2	-9.0	-10.5
α,4-dichlorotoluene	700-275-3	718-71-8	718718	3593	Reach_4835	2227	217	88.5	1.4E-02	7.4E+01	4.0E+02			3.5E-07	3.5E-08	1.1E-07				20%	-9.3	-9.0	-10.5

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
di-tert-butyl 1,1,4,4-tetramethyltetramethylene diperoxide	201-128-1	78-63-7	78637	3753	Reach_202	2228	290	64.9	1.3E+00	1.4E-01	3.5E+06			1.1E-06	1.1E-07	3.5E-07				22%	-9.2	-9.0	-11.7
619-846-2	256-462-0	49744-39-0	49744390	5895	Reach_2765	2229	348	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				17%	-9.2	-9.0	-10.8
4H-3,1-benzoxazine-2,4(1H)-dione	202-209-4	93-01-6	93016	4055	Reach_396	2230	224	173.0	4.1E-07	4.3E+03	3.4E-01	0.68		1.1E-06	1.1E-07	3.5E-07				14%	-9.0	-9.0	-10.9
camphene	201-234-8	79-92-5	79925	928	Reach_251	2231	136	-15.3	2.4E+02	1.8E+01	2.2E+04			2.1E-08	3.5E-08	3.5E-08				24%	-9.3	-9.0	-11.5
2-Butenoic acid, 4-oxo-4-(tridecylamino)-, (Z)-, branched	283-219-6	84583-68-6	84583686	3868	Reach_2976	2232	297	198.7	3.0E-07	2.8E+00	5.6E+05	3.92	15.2	1.1E-06	1.1E-07	3.5E-07				14%	-8.4	-9.0	-11.0
cyclohexyl isocyanate	212-958-9	887-76-3	887763	3964	Reach_1585	2233	250	274.2	3.4E-15	1.5E-02	7.8E-01			1.1E-06	1.1E-07	1.1E-06				15%	-9.3	-9.0	-10.5
8,9,10-trinorborn-2-ene	207-866-0	498-66-8	498668	650	Reach_1297	2234	94	-60.5	4.3E+03	2.1E+02	7.1E+02			2.6E-08	1.1E-07	3.5E-07				23%	-9.3	-9.0	-11.6
(1R)-6,6-dimethylbicyclo[3.1.1]hept-2-en-2-ethanol	252-744-2	35836-73-8	35836738	2751	Reach_2694	2235	166	49.6	6.3E-01	1.4E+03	1.9E+03	15.9		1.1E-06	3.5E-07	1.1E-06				15%	-9.3	-9.0	-10.9
N,N-dicyclohexylbenzothiazole-2-sulphenamide	204-683-8	124-13-0	124130	1786	Reach_1070	2236	128	-31.1	2.0E+02	5.0E+02	6.0E+02			1.1E-06	1.1E-07	3.5E-07				23%	-9.3	-9.0	-11.8
isosorbide dinitrate	201-740-9	87-33-2	87332	3926	Reach_308	2237	236	82.1	8.0E-02	4.5E+04	5.8E+00			1.1E-06	1.1E-07	3.5E-07				14%	-8.3	-9.0	-11.1
exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl methacrylate	231-403-1	7534-94-3	7534943	3668	Reach_2260	2238	222	54.1	1.4E+00	5.6E+01	5.8E+04			3.5E-06	3.5E-07	1.1E-06				16%	-9.3	-9.0	-10.7
4-tert-butylcyclohexanone	617-040-5	80286-58-4	80286584	3790	Reach_4445	2239	248	124.3	7.2E-04	4.5E+01	3.3E+05			1.1E-06	3.5E-07	1.1E-06				15%	-9.3	-9.0	-10.5
606-524-1	700-231-3	18162-90-8	18162908	2170	Reach_4814	2240	162	-35.1	5.7E+02	0.0E+00	2.4E+01	0		3.5E-06	3.5E-07	1.1E-06				17%	-8.4	-9.0	-10.7
(3R,5aS,6R,8aS,9R,12S,12aR)-3,6,9-trimethyloctahydro-3,12-ep	209-939-2	598-55-0	598550	3290	Reach_1403	2241	75	-47.1	7.3E+01	4.5E+05	3.1E-01			1.1E-06	3.5E-07	1.1E-06				14%	-8.5	-9.0	-10.9
(1S,4R,6R)-1-[(3E)-5-hydroxy-3-methylpent-3-en-1-yn-1-yl]-2,2,	700-075-6	218768-11-7	218768117	2309	Reach_4753	2242	242	142.2	1.4E-06	3.6E+03	2.6E+02	8.64		1.1E-06	3.5E-08	1.1E-07				14%	-8.2	-9.0	-10.9
cinnamaldehyde	203-213-9	104-55-2	104552	168	Reach_623	2243	132	0.0	4.5E+00	3.9E+02	6.6E+01			1.2E-06	3.5E-07	1.1E-06				14%	-9.3	-9.0	-10.6
2-ethylhexyl salicylate	204-263-4	118-60-5	118605	1675	Reach_967	2244	250	108.9	9.5E-04	2.3E+00	9.3E+05	9.8		1.1E-06	1.1E-07	3.5E-07				19%	-9.0	-9.0	-10.6
vinyltoluene	246-562-2	25013-15-4	25013154	2412	Reach_2557	2245	118	-30.1	2.8E+02	1.2E+02	2.8E+03			3.5E-07	3.5E-08	1.1E-07				20%	-9.3	-9.0	-11.2
1,2,3,4-tetrahydronaphthalene	204-340-2	119-64-2	119642	355	Reach_983	2246	132	-4.5	3.3E+01	2.4E+01	9.1E+03			2.4E-08	3.5E-08	1.1E-07				23%	-9.3	-9.0	-11.0
616-291-8	616-291-8	76114-73-3	76114733	3699	Reach_4431	2247	155	30.3	1.9E+01	7.8E+02	4.4E+01	12		3.5E-06	3.5E-07	1.1E-06				14%	-9.3	-9.0	-10.7
2-(4-methylpentan-2-yl)aniline	615-161-8	707-72-2	707722	3569	Reach_4412	2248	229	1.8	2.9E+01	2.9E+01	8.7E+03			3.5E-07	3.5E-08	1.1E-07				14%	-9.3	-9.0	-11.0
3-(triethoxysilyl)propyl prop-2-enoate	258-011-3	52567-96-1	52567961	3063	Reach_2783	2249	166	18.1	2.0E+00	1.1E+04	1.9E+03			1.1E-06	1.1E-07	3.5E-07				14%	-9.3	-9.0	-11.0
acetoacetamide	227-774-4	5977-14-0	5977140	3286	Reach_2146	2250	101	62.2	1.4E+00	3.1E+05	5.6E-02	8.9	14.3	1.1E-06	3.5E-07	1.1E-06				14%	-8.3	-9.0	-11.1
616-320-4	616-320-4	763105-70-0	763105700	3708	Reach_4434	2251	210	137.1	1.8E-03	1.9E+03	1.8E-01		4.03	1.1E-06	3.5E-07	1.1E-06				14%	-8.2	-9.0	-11.1
2-ethylhexyl acetate	203-079-1	103-09-3	103093	1359	Reach_601	2252	172	-20.5	5.1E+01	1.8E+02	5.5E+03			3.5E-06	3.5E-07	1.1E-06				15%	-9.3	-9.0	-11.0
tetradecanedioic acid	212-476-9	821-38-5	821385	3819	Reach_1554	2253	258	158.1	7.4E-05	4.7E+01	1.4E+04	4.6		1.1E-06	1.1E-07	3.5E-07				14%	-8.5	-9.0	-11.0
(E)-3-methylpent-2-en-4-yn-1-ol	690-510-5	5693-27-6	5693276	3216	Reach_4656	2254	162	85.7	1.5E-02	3.4E+03	4.6E+01			1.1E-06	1.1E-07	3.5E-07				14%	-9.3	-9.0	-10.9
(Z)-3-methylpent-2-en-4-yn-1-ol	611-622-2	581076-60-0	581076600	3241	Reach_4361	2255	368	236.4	9.5E-10	1.7E+01	1.3E+03	14.2		1.1E-06	3.5E-08	1.1E-07				14%	-9.3	-9.0	-10.9
2,4,6,8,10-pentamethylcyclopentasiloxane	228-204-7	6166-86-5	6166865	3347	Reach_2156	2256	296	-21.6	2.2E+02	1.2E+03	1.6E+05			3.5E-09	3.5E-09	3.5E-09				24%	-9.3	-9.0	-10.8
2-ethylhexyl chloroformate	246-278-9	24468-13-1	24468131	2395	Reach_2547	2257	193	-8.3	3.4E+01	3.2E+01	3.2E+03			3.5E-06	3.5E-07	1.1E-06				16%	-9.3	-9.0	-11.5
3-[methoxy(dimethyl)silyl]propan-1-amine	207-256-4	456-04-2	456042	2944	Reach_1280	2258	173	25.4	6.8E+00	1.6E+03	1.3E+02			1.1E-06	3.5E-07	1.1E-06				14%	-9.3	-9.0	-10.7
stearamide	204-693-2	124-26-5	124265	1789	Reach_1074	2259	284	152.0	8.9E-05	3.4E-03	5.0E+06	15.1	14.3	1.1E-06	1.1E-07	3.5E-07				21%	-9.1	-9.0	-10.4
1-[4-(trans-4-propylcyclohexyl)phenyl]butan-1-one	639-407-9	201733-56-4	201733564	2252	Reach_4604	2260	226	50.7	2.7E+00		7.8E-01			3.5E-07	1.1E-07	3.5E-07				21%	-8.8	-9.0	-10.4
4,4'-diamino[1,1'-bianthracene]-9,9',10,10'-tetraone	223-754-4	4051-63-2	4051632	2858	Reach_2007	2261	444	317.3	2.6E-15	7.2E-02	6.8E+06		13.5	1.1E-06	3.5E-07	1.1E-06				15%	-8.3	-9.0	-10.9
N,N'-1,4-phenylenebis[3-oxobutyramide]	246-438-8	24731-73-5	24731735	2402	Reach_2554	2262	276	220.6	1.1E-08	1.1E+04	1.0E+00	10.4	13.1	1.1E-06	3.5E-07	1.1E-06				14%	-7.9	-9.0	-11.0
2-cyano-N-methylacetamide	690-730-1	486460-32-6	486460326	2974	Reach_4660	2263	407	181.6	3.9E-06	5.6E+00	2.5E+01	0		1.1E-07	3.5E-08	1.1E-07				14%	-8.2	-9.0	-11.2
3-α-hydroxy-7-oxo-5-β-cholan-24-oic acid	238-883-1	14814-09-6	14814096	2001	Reach_2370	2264	238	36.5	1.0E+00	3.3E+02	5.4E+01	10.2		3.5E-07	1.1E-07	3.5E-07				15%	-8.4	-9.0	-10.9
acetyl chloride	200-865-6	75-36-5	75365	858	Reach_141	2265	78	-80.5	4.0E+04	5.6E+04	3.4E-01			4.5E-06	1.1E-07	3.5E-07				14%	-9.4	-9.0	-11.4
7-oxabicyclo[4.1.0]hept-3-ylmethyl 7-oxabicyclo[4.1.0]heptane	219-207-4	2386-87-0	2386870	2362	Reach_1792	2266	252	91.7	8.0E-02	1.1E+03	2.3E+02			3.5E-06	3.5E-07	1.1E-06				14%	-9.2	-9.0	-10.9
hexadecyl 2-ethylhexanoate	204-493-5	121-69-7	121697	373	Reach_1018	2267	121	-24.6	6.7E+01	1.4E+04	1.5E+02			1.4E-08	1.1E-07	3.5E-07				24%	-9.2	-9.0	-9.9
tris(2-chloroethyl) phosphate	700-177-0	467430-13-3	467430133	5892	Reach_4792	2268	679	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				22%	-9.3	-9.0	-10.1
620-343-5	611-624-3	581076-67-7	581076677	5939	Reach_4362	2269	417	0.0												15%	-9.3	-9.0	-10.5
1-ethynylcyclohexanol	288-270-8	85702-79-0	85702790	3896	Reach_2987	2270	271	182.0	3.3E-06	5.6E+01	7.8E+03	4.87		1.1E-06	1.1E-07	3.5E-07				23%	-9.3	-9.0	-10.2
linalyl acetate	204-116-4	115-95-7	115957	1640	Reach_947	2271	196	-2.1	1.7E+01	3.6E+02	2.5E+04			3.5E-06	3.5E-07	1.1E-06				16%	-9.3	-9.0	-10.7
1,4-dihydroxyanthraquinone	229-942-2	6850-63-1	6850631	801	Reach_2208	2272	127	-11.1	1.6E+02	5.7E+01	3.0E+02			2.6E-07	3.5E-08	1.1E-07				15%	-8.2	-9.0	-10.9
3,5,5-trimethylhexan-1-ol	222-376-7	3452-97-9	3452979	609	Reach_1964	2273	144	-18.7	1.4E+01	1.2E+02	1.3E+03	15.9		1.4E-07	1.1E-06	3.5E-06				19%	-9.3	-9.0	-10.5
616-123-3	616-123-3	746595-79-9	746595799	3641	Reach_4423	2274	102	25.5	6.4E+01	8.8E+06	1.2E-01		7.48	1.1E-06	1.1E-07	3.5E-07				14%	-8.2	-9.0	-11.2
methyl 3-oxovalerate	202-299-5	94-05-3	94053	4097	Reach_411	2275	169	29.6	1.4E+00	8.7E+03	1.1E+01			3.5E-06	3.5E-07	1.1E-06				14%	-9.3	-9.1	-10.9
chloroacetone	201-161-1	78-95-5	78955	3761	Reach_218	2276	93	-59.2	2.2E+03	3.8E+04	1.0E+00			3.5E-07	3.5E-08	1.1E-07				16%	-9.4	-9.1	-10.5
O,O-diisopropyl hydrogen dithiophosphate	221-496-7	3120-74-9	3120749	2620	Reach_1918	2277	154	57.1	3.7E-01	3.4E+03	4.6E+02	9.5		1.1E-05	1.1E-06	3.5E-06				17%	-9.3	-9.1	-10.4
nerol	203-378-7	106-25-2	106252	187	Reach_662	2278	154	-10.8	2.1E+00	3.4E+02	3.0E+03	15.5		5.8E-07	3.5E-07	1.1E-06				16%	-9.3	-9.1	-10.6
3-methoxyandrosta-3,5-dien-17-one	220-371-4	2741-57-3	2741573	2505	Reach_1861	2279	278	68.5	1.9E-01	2.8E+00	7.6E+04			3.5E-07	3.5E-08	1.1E-07				17%	-9.3	-9.1	-10.8
dodecane-1-thiol	203-984-1	112-55-0	112550	1592	Reach_913	2280	202	15.7	9.9E-01	2.5E-02	1.5E+06	10.7		3.5E-07	3.5E-08	1.1E-07				23%	-9.3	-9.1	-11.7
(epoxyethyl)benzene	202-476-7	96-09-3	96093	1044	Reach_450	2281	120	-15.7	6.5E+01	4.0E+03	3.9E+01			7.4E-07	3.5E-08	1.1E-07				15%	-9.3	-9.1	-10.5
methyl isothiocyanate	209-132-5	556-61-6	556616	704	Reach_1367	2282	73	-63.3	1.6E+03	6.6E+03	2.0E+01			5.4E-09	3.5E-07	1.1E-06				23%	-9.3	-9.1	-10.6
2,2'-[ethane-1,2-diylbis(oxy)]bisethyl diacetate	203-846-0	111-21-7	111217	1542	Reach_849	2283	234	-15.8	5.5E-01	5.1E+04	7.2E-01			3.5E-06	3.5E-07	1.1E-06				14%	-8.8	-9.1	-11.2
p-phenylbenzaldehyde	221-742-3	3218-36-8	3218368	2644	Reach_1934	2284	182	73.1	2.5E-02	1.3E+01	3.0E+03			3.5E-07	3.5E-08	3.5E-08				17%	-9.3	-9.1	-10.7
4-(trifluoromethoxy)aniline	207-317-5	461-82-5	461825	2949	Reach_1284	2285	177	26.7	2.5E+01	5.5E+02	1.3E+02		10.3	1.1E-06	1.1E-07	3.5E-07				14%	-8.9	-9.1	-11.0
(1-hydroxyethylidene)bisphosphonic acid, potassium salt	267-956-0	67953-76-8	67953768	5990	Reach_2893	2286	358	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.7	-9.1	-10.7
exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acetate	204-727-6	125-12-2	125122	1796	Reach_1083	2287	196	34.1	1.4E+01	3.8E+02	7.2E+03			3.5E-06	3.5E-07	1.1E-06				15%	-9.3	-9.1	-10.7
trichloro(propyl)silane	205-489-6	141-57-1	141571	1936	Reach_1164	2288	178	-51.4	1.8E+03	8.9E+03	9.8E+02			1.1E-06	3.5E-07	1.1E-06				15%	-9.3	-9.1	-10.9
800-181-3	204-018-1	112-95-8	112958	1613	Reach_931	2289	283	51.8	4.1E-02	1.1E-04	1.4E+10									18%	-8.7	-9.1	-10.7
manganese oxalate	211-367-3	640-67-5	640675	5965	Reach_1478	2290	143	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.8	-9.1	-10.7
isobutyl vinyl ether	203-678-8	109-53-5	109535	1501	Reach_775	2291	100	-88.5	1.1E+04	4.4E+03	6.6E+01			1.1E-06	3.5E-07	1.1E-06				17%	-9.4	-9.1	-11.4
2-allyloxymethyl-2-ethylpropanediol	211-662-7	682-11-1	682111	3511	Reach_1500	2292	174	57.4	1.4E-02	8.5E+03	5.4E+00	14.9		1.1E-06	1.1E-07	3.5E-07				14%	-8.3	-9.1	-11.1
2,6-diisopropylphenyl isocyanate	201-869-0	88-95-9	88959	3965	Reach_334	2293	203	68.2	7.1E-01	7.2E+02	7.6E+00			3.5E-06	3.5E-07	1.1E-06				20%	-9.3	-9.1	-10.6
2-methylbutene	247-975-0	26760-64-5	26760645	2486	Reach_2592	2294	70	-117.4	8.1E+04	6.0E+02	5.2E+02			3.5E-07	1.1E-07	3.5E-07				22%	-9.4	-9.1	-11.9
2,3,7,8-tetrahydro-2,5,8-benzotrioxacycloundecine-1,9-dione	205-491-7	141-62-8	141628	1939	Reach_1165	2295	311	-36.3	6.5E+01	2.4E-02	1.4E+08			3.5E-09	3.5E-09	3.5E-09				14%	-8.2	-9.1	-11.1
α,2,2,6-tetramethylcyclohexene-1-butyraldehyde	206-524-8	352-70-5	352705	2727	Reach_1243	2296	110	-54.2	2.6E+03	4.9E+02	5.5E+02			3.5E-07	3.5E-08	1.1E-07				19%	-9.3	-9.1	-10.4
propionic anhydride	204-638-2	123-62-6	123626	1772	Reach_1054	2297	130	-69.3	2.1E+02	1.3E+04	2.5E+00			3.5E-06	3.5E-07	1.1E-06				14%	-9.3	-9.1	-10.8
p-menth-1-en-8-ol	202-680-6	98-55-5	98555	1074	Reach_512	2298	154	12.4	2.6E+00	3.8E+03	2.1E+03	16		6.4E-07	1.1E-07	3.5E-07				16%	-9.3	-9.1	-10.9
1,2,3-trichlorobenzene	207-677-3	488-43-7	488437	2977	Reach_1293	2299	181	132.8	2.2E-06	1.0E+06	2.5E-04			3.5E-06	1.1E-06	3.5E-06				24%	-9.4	-9.1	-10.8
2-chloro-1,1-dimethoxyethane	202-751-1	99-34-3	99343	4204	Reach_527	2300	212	147.9	4.1E-05	3.8E+03	3.2E+01			1.1E-06	3.5E-08	1.1E-07				16%	-9.4	-9.1	-10.5
2-methyl-6-methyleneoct-7-en-2-ol	208-843-8	543-39-5	543395	3138	Reach_1349	2301	154	-12.0	1.2E+01	3.8E+02	2.9E+03	16		1.1E-06	1.1E-07	3.5E-07				15%	-9.3	-9.1	-10.5
trazodone	203-913-4	111-84-2	111842	1560	Reach_875	2302	128	-56.2	6.6E+02	1.5E+00	5.8E+04		0	3.5E-07	3.5E-08	1.1E-07				15%	-8.4	-9.1	-11.0

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
3,3-bis[(dimethylvinylsilyl)oxy]-1,1,5,5-tetramethyl-1,5-divinyltr	262-061-1	60111-54-8	60111548	3304	Reach_2843	2303	433	11.6	6.8E-01	0.0E+00	1.1E+11			1.1E-06	1.1E-07	3.5E-07				24%	-9.3	-9.1	-10.1
octane-1-thiol	203-918-1	111-88-6	111886	1563	Reach_879	2304	146	-28.3	5.0E+01	2.6E+01	1.6E+04	10.7		1.1E-06	1.1E-07	3.5E-07				18%	-9.4	-9.1	-11.3
2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2-me	224-867-1	4531-49-1	4531491	2939	Reach_2046	2305	690	349.8	5.8E-21	8.6E-05	1.2E+06	8.45	13.7	3.5E-07	3.5E-08	3.5E-08				21%	-8.2	-9.1	-10.4
605-152-7	212-562-6	826-81-3	826813	3836	Reach_1558	2306	159	94.4	2.0E-01	2.1E+03	1.6E+02			3.5E-06	3.5E-07	1.1E-06				17%	-9.3	-9.1	-10.8
exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acrylate	227-561-6	5888-33-5	5888335	3257	Reach_2140	2307	208	43.9	1.0E+00	8.7E+01	1.6E+04			3.5E-06	3.5E-07	1.1E-06				15%	-9.3	-9.1	-10.8
3-cyclohexylpropionic acid	211-861-9	701-97-3	701973	3557	Reach_1516	2308	156	57.9	8.6E-01	5.1E+02	2.2E+03	4.9		1.1E-06	1.1E-07	3.5E-07				14%	-8.9	-9.1	-11.1
N,N-dimethyl-3-oxobutyramide	218-059-8	2044-64-6	2044646	2265	Reach_1750	2309	129	31.7	1.4E+01	6.1E+06	2.6E-01	8.9	14.3	1.1E-06	3.5E-07	1.1E-06				14%	-8.4	-9.1	-11.1
phenyl acetate	204-575-0	122-79-2	122792	382	Reach_1035	2310	136	-11.9	5.9E+01	2.5E+03	3.9E+01			7.2E-07	3.5E-07	1.1E-06				15%	-9.3	-9.1	-10.5
heptan-2-ol	201-947-4	89-87-2	89872	3988	Reach_354	2311	151	53.2	4.3E+00	1.2E+02	8.1E+02			3.5E-06	3.5E-08	1.1E-07				15%	-9.3	-9.1	-10.5
hexahydro-4-methylphthalic anhydride	243-072-0	19438-60-9	19438609	2232	Reach_2480	2312	168	5.4	4.4E+00	1.5E+01	3.9E+02			3.5E-06	3.5E-07	1.1E-06				15%	-9.4	-9.1	-11.0
800-696-3	800-696-3	78605-96-6	78605966	3752	Reach_5047	2313	202	33.9	6.0E-02	8.6E+00	2.1E+04			1.1E-06	1.1E-07	3.5E-07				16%	-9.3	-9.1	-10.7
1,1'-(methylimino)dipropan-2-ol	224-536-1	4402-30-6	4402306	2919	Reach_2032	2314	147	21.9	6.7E-01	1.0E+06	2.1E-01	14.7	5	3.5E-06	1.1E-06	3.5E-06				14%	-8.2	-9.1	-11.1
diethyl 1,2-cyclopentanedicarboxylate	213-107-4	924-50-5	924505	4034	Reach_1594	2315	114	-66.1	1.2E+02	8.5E+03	4.9E+01			3.5E-06	3.5E-07	1.1E-06				14%	-9.3	-9.1	-11.0
4-[(morpholinothio)thioxomethyl]morpholine	205-439-3	140-89-6	140896	1195	Reach_1152	2316	160	0.0	0.0E+00	0.0E+00	0.0E+00		0	0.0E+00	0.0E+00	0.0E+00				14%	-8.0	-9.1	-11.2
sodium p-(3-amino-4-methylbenzamido)benzenesulphonate	201-899-4	89-33-8	89338	3971	Reach_340	2317	232	143.0	2.1E-04	2.6E+05	1.3E+02									18%	-8.8	-9.1	-10.8
methyl (R)-amino(4-hydroxyphenyl)acetate	202-870-9	100-61-8	100618	133	Reach_564	2318	107	-20.7	5.8E+01	2.6E+03	4.2E+01		9	5.8E-09	1.1E-07	3.5E-07				14%	-8.1	-9.1	-11.0
mucochloric acid	201-752-4	87-56-9	87569	3935	Reach_310	2319	169	58.7	1.4E-01	6.4E+04	2.3E+01	0.69		1.1E-06	1.1E-07	3.5E-07				14%	-8.2	-9.1	-11.1
2,2-Dichloro-1-(3-methyl-2,3-dihydro-4H-1,4-benzoxazin-4-yl)e	202-548-8	96-97-9	96979	4158	Reach_473	2320	183	147.0	1.7E-05	7.0E+03	4.4E+02			3.5E-06	1.1E-07	3.5E-07				16%	-9.0	-9.1	-10.9
bis[2-[2-(2-butoxyethoxy)ethoxy]ethyl] adipate	265-807-4	65520-46-9	65520469	3455	Reach_2874	2321	523	191.5	3.3E-08	4.5E-01	4.9E+02			1.1E-06	1.1E-07	3.5E-07				15%	-8.4	-9.1	-11.0
N,N,N',N'-tetramethyltrimethylenediamine	203-818-8	110-95-2	110952	1533	Reach_839	2322	130	-35.3	7.1E+02	3.2E+04	1.7E+00		4.4	1.1E-06	1.1E-07	1.1E-06				14%	-9.3	-9.1	-10.6
oxiniacic acid	216-676-7	1638-86-4	1638864	2090	Reach_1702	2323	198	26.4	1.9E+00	1.7E+02	1.5E+02	0	0	3.5E-07	3.5E-08	1.1E-07				14%	-8.1	-9.1	-11.3
hexadecyl acrylate	236-492-0	13402-02-3	13402023	1875	Reach_2334	2324	297	80.5	5.8E-03	6.3E-03	1.2E+08			1.1E-06	1.1E-07	3.5E-07				23%	-9.0	-9.1	-10.8
propylphosphonic dichloride	202-685-3	98-60-2	98602	4189	Reach_515	2325	211	85.1	1.6E-01	5.2E+02	3.9E+03			1.1E-07	1.1E-08	3.5E-08				14%	-9.3	-9.1	-10.6
(+)-L-arginine hydrochloride	206-200-6	307-35-7	307357	2611	Reach_1232	2326	502	27.2	7.7E+02	7.9E-02	6.9E+07									18%	-8.8	-9.1	-10.8
1,3-di-o-tolylguanidine	202-577-6	97-39-2	97392	4164	Reach_478	2327	239	142.2	6.9E-05	5.5E+00	9.8E+03		3.9	1.1E-06	3.5E-08	1.1E-07				16%	-9.0	-9.1	-11.0
OO-tert-butyl O-(2-ethylhexyl) peroxycarbonate	252-029-5	34443-12-4	34443124	2706	Reach_2678	2328	246	-4.3	5.7E-01	7.7E+01	4.6E+04			3.5E-06	3.5E-07	1.1E-06				16%	-9.3	-9.1	-10.9
(R)-1-hydroxy-1-phenylacetone	210-676-0	621-29-4	621294	3362	Reach_1442	2329	133	-19.2	1.3E+02	2.3E+03	1.4E+03	0		1.1E-06	3.5E-07	1.1E-06				14%	-8.5	-9.1	-11.1
3-hydroxy-2'-methoxy-2-naphthanilide	205-206-6	135-62-6	135626	1894	Reach_1133	2330	293	216.3	2.6E-09	1.3E+01	9.8E+03	10.2		3.5E-07	3.5E-08	1.1E-07				17%	-8.4	-9.1	-10.8
3-(p-tert-butylphenyl)-2-methylpropanol	223-786-9	4073-98-7	4073987	2864	Reach_2010	2331	254	162.9	2.0E-05	6.8E+00	2.3E+04	0		3.5E-07	3.5E-08	1.1E-07				18%	-9.3	-9.1	-10.8
valeronitrile	203-781-8	110-59-8	110598	1523	Reach_818	2332	83	-46.1	8.0E+02	1.5E+04	2.1E+01			3.5E-07	3.5E-08	1.1E-07				16%	-9.4	-9.1	-10.4
O,O,O-tris(4-nitrophenyl) thiophosphate	222-314-9	3423-25-4	3423254	2696	Reach_1957	2333	169	44.4	3.4E-01	1.3E+04	1.4E+01			1.1E-06	3.5E-07	1.1E-06				19%	-9.1	-9.1	-10.9
diethyl carbonate	203-311-1	105-58-8	105588	179	Reach_644	2334	118	-95.3	1.6E+03	4.2E+04	1.7E+01			1.2E-06	1.1E-07	3.5E-07				15%	-9.4	-9.1	-10.6
isopentyl acetate	204-662-3	123-92-2	123922	398	Reach_1061	2335	130	-56.1	7.6E+02	3.5E+03	1.8E+02			5.1E-07	3.5E-07	1.1E-06				16%	-9.4	-9.1	-10.7
chloro(methyl)silane	213-600-4	993-00-0	993000	4201	Reach_1626	2336	81	-119.2	3.8E+05		2.5E+01			3.5E-09	3.5E-09	3.5E-09				24%	-9.7	-9.1	-11.7
methyl benzoate	202-259-7	93-58-3	93583	4073	Reach_403	2337	136	-11.9	5.1E+01	2.1E+03	6.8E+01			3.5E-06	3.5E-07	1.1E-06				14%	-9.4	-9.1	-10.7
2-ethylanthraquinone	201-535-4	84-51-5	84515	3867	Reach_285	2338	236	146.5	3.6E-04	1.2E-01	2.4E+04			1.1E-06	1.1E-07	3.5E-07				16%	-9.3	-9.1	-10.9
ethyldiisopropylamine	230-392-0	7087-68-5	7087685	814	Reach_2225	2339	129	-68.8	1.6E+03	1.3E+04	2.2E+02		3	7.8E-08	1.1E-07	3.5E-07				20%	-9.4	-9.1	-10.6
601-327-7	605-152-7	15854-73-6	15854736	2063	Reach_4169	2340	229	125.9	8.0E-04	2.3E+00	4.6E+03			3.5E-07	1.1E-07	3.5E-07				17%	-9.3	-9.1	-10.8
Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo	237-331-7	13749-61-6	13749616	1909	Reach_2348	2341	127	47.4	2.3E+00	7.5E+03	1.3E+01	15.1	14.4	1.1E-06	3.5E-07	1.1E-06				23%	-8.8	-9.1	-9.9
Disodium hydroxy(sulfonato)acetate	608-408-6	29736-24-1	29736241	5824	Reach_4275	2342	178	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.8	-9.1	-10.8
3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-indene	224-778-8	4488-57-7	4488577	2933	Reach_2040	2343	134	-18.0	2.3E+02	8.8E+02	2.4E+03			1.1E-06	1.1E-07	3.5E-07				16%	-9.4	-9.1	-10.8
1,6-dichlorohexane	264-840-1	64354-92-3	64354923	3434	Reach_2865	2344	211	48.2	1.7E-01	1.0E+01	8.5E+03			3.5E-07	3.5E-08	1.1E-07				18%	-9.4	-9.1	-10.7
N-isopropylmethacrylamide	290-824-9	90268-24-9	90268249	3996	Reach_2992	2345	752	349.8	3.9E-22	1.7E-06	6.8E+07	8.45	13.7	1.1E-07	1.1E-08	1.1E-08				14%	-9.4	-9.1	-11.0
oxydiethylene dibenzoate	204-407-6	120-55-8	120558	1714	Reach_997	2346	314	59.8	1.1E+01	7.2E+01	1.1E+03			1.1E-06	1.1E-07	3.5E-07				16%	-9.4	-9.1	-11.0
(1R)-1-[(4R,4aR,8aS)-2,6-bis(4-chlorophenyl)tetrahydro[1,3]dio	200-541-4	62-55-5	62555	766	Reach_65	2347	75	-21.0	2.4E+02	1.5E+05	1.5E-01	13.4		2.9E-09	3.5E-07	1.1E-06				23%	-8.3	-9.1	-10.2
2,2-dichloro-1,1,1-trifluoroethane	206-190-3	306-83-2	306832	2607	Reach_1231	2348	153	-99.6	9.4E+04	1.7E+03	1.5E+02			3.5E-08	1.1E-08	1.1E-08				23%	-9.7	-9.1	-11.8
1-phenylethyl hydroperoxide	254-639-7	39811-17-1	39811171	2849	Reach_2728	2349	199	109.7	2.5E-03	5.0E+01	8.3E+02	0		3.5E-07	1.1E-07	1.1E-07				16%	-9.4	-9.1	-10.7
3-[(2-hydroxyethyl)amino]propionamide	248-211-9	27076-30-8	27076308	2494	Reach_2597	2350	132	112.0	5.3E-04	1.0E+05	2.2E-03	14.2	5.22	3.5E-06	1.1E-06	3.5E-06				14%	-8.1	-9.1	-11.2
tripotassium propylsilanetriolate	201-919-1	89-57-6	89576	3980	Reach_345	2351	153	128.9	8.1E-06	1.4E+04	9.5E+00									18%	-8.8	-9.1	-10.8
1,1'-[oxybis(ethyleneoxy)]diethylene	201-708-4	86-92-0	86920	3913	Reach_305	2352	188	124.7	2.6E-03	1.1E+03	1.3E+03			1.1E-06	3.5E-07	1.1E-06				16%	-9.4	-9.1	-10.5
3-methyl-1-p-tolyl-5-pyrazolone	240-241-0	16088-62-3	16088623	498	Reach_2411	2353	58	-100.2	7.1E+04	5.8E+04	2.3E+00			6.1E-07	1.1E-07	3.5E-07				15%	-8.7	-9.1	-11.0
2-[2-(3-aminopropoxy)ethoxy]ethanol	610-513-7	502421-44-5	502421445	2998	Reach_4331	2354	424	292.1	1.5E-13	2.5E+02	4.2E+01	9.32	11.8	1.1E-06	1.1E-07	1.1E-06				14%	-8.1	-9.1	-11.2
608-271-2	608-271-2	28861-00-9	28861009	2547	Reach_4268	2355	282	189.7	1.2E-06	3.5E+03	6.5E+00	3.82	14.8	1.1E-06	1.1E-07	3.5E-07				14%	-8.0	-9.1	-11.2
3,5,5-trimethylhexanoyl chloride	253-168-4	36727-29-4	36727294	2775	Reach_2703	2356	177	-10.9	1.6E+02	3.0E+00	6.0E+02			1.1E-06	3.5E-07	1.1E-06				20%	-9.4	-9.1	-12.1
1,3-benzodioxolane	205-992-0	274-09-9	274099	2504	Reach_1218	2357	122	3.7	1.9E+02	3.7E+02	1.1E+02			1.1E-06	3.5E-07	1.1E-06				16%	-9.4	-9.1	-11.0
N-[[(4-methylphenyl)sulfonyl]methyl]formamide	607-301-1	23996-53-4	23996534	2364	Reach_4236	2358	121	77.0	8.7E-02	4.7E+04	1.3E+00	0		3.5E-07	3.5E-08	1.1E-07				14%	-8.1	-9.1	-11.3
2-ethylhexyl methacrylate	211-708-6	688-84-6	688846	3529	Reach_1504	2359	198	-7.8	1.0E+01	2.8E+01	4.4E+04			3.5E-06	3.5E-07	1.1E-06				17%	-9.4	-9.1	-11.2
N-ethyl-N-[2-[1-(2-methylpropoxy)ethoxy]ethyl]-4-(phenylazo).	204-129-5	116-16-5	116165	1647	Reach_953	2360	265	36.2	4.1E+01	1.8E+01	3.0E+02		0	3.5E-08	1.1E-08	3.5E-08				14%	-8.6	-9.1	-11.1
3-[(2-Ammonio-4,5-dimethoxyphenyl)diazenyl]-4-methoxyben:	226-323-9	5351-04-2	5351042	1274	Reach_2102	2361	126	-0.4	3.7E+01	4.5E+04	3.4E+00	0	6.4	1.1E-06	3.5E-07	1.1E-06				14%	-8.0	-9.1	-11.2
1-methylpiperidine	230-262-3	6994-25-8	6994258	3553	Reach_2218	2362	155	106.7	9.7E-03	3.6E+04	3.0E-01		12.7	3.5E-06	3.5E-07	1.1E-06				23%	-9.4	-9.1	-10.5
N-[3-(dimethylamino)propyl]formamide	227-652-0	5922-69-0	5922690	3269	Reach_2144	2363	130	68.2	5.9E-01	1.0E+06	1.1E-01	14.8	4.56	3.5E-06	3.5E-07	3.5E-06				14%	-8.3	-9.1	-11.2
[1,3-phenylenebis(1-methylethylidene)]bis[tert-butyl] peroxide	218-664-7	2212-81-9	2212819	2320	Reach_1772	2364	338	113.3	2.3E-03	5.4E-02	2.2E+07			3.5E-07	3.5E-08	1.1E-07				23%	-9.2	-9.1	-10.3
octane-1,2-diol	214-254-7	1117-86-8	1117868	1557	Reach_1651	2365	146	23.8	2.2E-01	4.0E+03	4.7E+01	14.9		3.5E-06	1.1E-06	3.5E-06				14%	-9.2	-9.1	-11.0
diisopropyl 3,3'-[(2,5-dichloro-1,4-phenylene)bis[iminocarbony	262-062-7	60113-43-1	60113431	3305	Reach_2844	2366	166	19.5	2.1E+01	4.0E+02	1.9E+03	0		1.1E-06	3.5E-07	1.1E-06				24%	-9.4	-9.1	-8.0
1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthyl)ethan	216-133-4	1506-02-1	1506021	2011	Reach_1688	2367	258	106.9	2.5E-02	6.1E-01	2.2E+06			3.5E-07	3.5E-08	1.1E-07				21%	-9.3	-9.1	-10.4
1-[2-amino-1-(4-methoxyphenyl)ethyl]cyclohexanol hydrochlor	603-392-7	130198-05-9	130198059	5658	Reach_4118	2368	286	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.8	-9.1	-10.8
bis(1,2,2,6,6-pentamethyl-4-piperidyl) [[3,5-bis(1,1-dimethyleth	264-513-3	63843-89-0	63843890	3419	Reach_2863	2369	685	277.7	9.5E-14	8.9E-06	1.1E+10	11.8	4.63	1.1E-06	1.1E-07	3.5E-07				23%	-9.1	-9.1	-9.7
2-amino-2-ethylpropanediol	204-101-2	115-70-8	115708	1638	Reach_943	2370	119	46.6	2.6E-01	1.0E+06	2.5E-01	14.4	5.2	3.5E-06	1.1E-06	3.5E-06				14%	-8.3	-9.1	-11.1
palmitoyl chloride	203-996-7	112-67-4	112674	1597	Reach_918	2371	275	77.0	1.2E-01	1.3E-02	2.5E+06			1.1E-06	1.1E-07	3.5E-07				22%	-9.4	-9.1	-11.8
1,2,3,6-tetrahydromethyl-3,6-methanophthalic anhydride	246-644-8	25134-21-8	25134218	2417	Reach_2559	2372	178	38.9	1.9E+00	4.2E+03	2.0E+02			3.5E-06	3.5E-07	1.1E-06				14%	-9.4	-9.1	-11.0
Methyl 1,3,3-trimethyl-2-methylidene-2,3-dihydro-1H-indole-5	700-542-4	917392-54-2	917392542	4020	Reach_4929	2373	320	189.8	1.2E-06	2.9E+01	3.3E+04			1.1E-06	1.1E-07	3.5E-07				17%	-9.3	-9.1	-10.8
ethanesulphonyl chloride	223-684-4	4023-34-1	4023341	2855	Reach_2006	2374	105	-44.7	3.7E+03	1.6E+04	2.1E+00			1.1E-06	3.5E-07	1.1E-06				14%	-9.4	-9.1	-10.9
undecan-1-ol	203-970-5	112-42-5	112425	329	Reach_906	2375	172	18.7	6.8E-01	2.0E+01	1.9E+04	15.9		3.7E-06	1.1E-07	3.5E-07				16%	-9.4	-9.1	-10.8
bis(2-ethoxyethyl) ether	230-625-6	7226-23-5	7226235	3600	Reach_2231	2376	128	28.5	1.5E+01	6.9E+04	1.5E+00			1.1E-06	1.1E-07	3.5E-07				15%	-9.4	-9.1	-11.1
3,3'-dimethoxybiphenyl-4,4'-ylenediammonium dichloride	235-464-5	12236-64-5	12236645	1748	Reach_2308	2377	502	349.8	8.7E-21	1.1E-01	6.2E+05									18%	-8.8	-9.1	-10.8

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
tetrahydro-1,3-dimethyl-1H-pyrimidin-2-one	221-659-2	3179-63-3	3179633	2636	Reach_1928	2378	103	-27.4	8.4E+01	9.6E+05	3.6E-01		4.8	3.5E-06	1.1E-06	3.5E-06				14%	-9.4	-9.1	-11.2
hydroxyprogesterone acetate	206-119-6	302-23-8	302238	2588	Reach_1229	2379	373	184.3	2.6E-06	2.3E+01	4.7E+03			3.5E-07	3.5E-08	1.1E-07				17%	-8.5	-9.2	-10.9
7-methyl-3-methyleneocta-1,6-diene	204-622-5	123-35-3	123353	390	Reach_1046	2380	136	-64.8	3.2E+02	1.1E+01	7.6E+04			4.4E-07	1.1E-07	3.5E-07				22%	-9.4	-9.2	-11.9
2-chloro-4-nitrotoluene	211-631-8	676-83-5	676835	3499	Reach_1496	2381	117	-87.4	2.2E+04	6.2E+03	6.3E+01			3.5E-09	3.5E-09	3.5E-09				23%	-9.4	-9.2	-10.3
7-acetamido-4-hydroxy-3-[[4-[[2-(sulphooxy)ethyl]sulphonyl]pl	287-574-8	85536-87-4	85536874	6061	Reach_2986	2382	618	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.8	-9.2	-10.8
Ethyl 3-oxo-3-(2,3,4,5-tetrafluorophenyl)propanoate	226-984-3	5586-73-2	5586732	3181	Reach_2128	2383	211	92.4	1.3E-02	5.3E+00	1.5E+03			1.1E-06	1.1E-07	3.5E-07				14%	-9.4	-9.2	-11.0
dioctyl ether	211-112-6	629-82-3	629823	3392	Reach_1471	2384	242	28.8	1.1E+00	7.2E-02	8.7E+06			1.1E-06	1.1E-07	3.5E-07				22%	-9.3	-9.2	-11.8
1,1,1,2,3,3,3-heptafluoropropane	207-079-2	431-89-0	431890	2907	Reach_1271	2385	170	-152.9	4.1E+05	4.5E+00	3.2E+02			3.5E-08	1.1E-08	3.5E-08				23%	-9.5	-9.2	-11.9
[[p-(2-methoxyethyl)phenoxy]methyl]oxirane	221-877-8	3266-23-7	3266237	2657	Reach_1938	2386	72	-91.3	3.2E+04	8.8E+04	6.2E+00			1.1E-06	3.5E-07	1.1E-06				14%	-9.4	-9.2	-11.1
6-tert-butyl-2,4-xylenol	217-533-1	1879-09-0	1879090	2209	Reach_1730	2387	178	66.5	1.6E+00	2.5E+02	3.3E+04	12.1		1.1E-06	1.1E-07	3.5E-07				17%	-9.4	-9.2	-10.7
bis(2-butoxyethyl) ether	204-001-9	112-73-2	112732	1600	Reach_921	2388	218	29.1	4.3E+00	7.9E+03	2.9E+02			1.1E-06	1.1E-07	3.5E-07				15%	-9.4	-9.2	-11.0
1,1,3,3-tetramethyldisiloxane	221-906-4	3277-26-7	3277267	2662	Reach_1940	2389	132	-110.6	5.3E+03	7.4E+02	1.4E+04			3.5E-09	3.5E-09	3.5E-09				24%	-9.6	-9.2	-11.7
methyl 5-deoxy-2,3-O-isopropylidene-β-D-ribofuranoside	208-859-5	544-10-5	544105	3142	Reach_1352	2390	121	-60.2	1.1E+03	6.9E+01	3.5E+03			1.1E-06	1.1E-07	3.5E-07				16%	-9.4	-9.2	-10.8
4-tert-butyltoluene	202-675-9	98-51-1	98511	1071	Reach_508	2391	148	-10.2	7.9E+01	9.3E+00	2.8E+04			4.5E-08	3.5E-08	1.1E-07				23%	-9.5	-9.2	-11.6
tert-butyl methacrylate	209-548-7	585-07-9	585079	3248	Reach_1385	2392	142	-47.9	8.2E+02	4.5E+03	4.4E+02			1.1E-06	3.5E-07	1.1E-06				15%	-9.4	-9.2	-10.8
Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo	609-057-1	35052-92-7	35052927	5854	Reach_4287	2393	239	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				16%	-8.9	-9.2	-11.1
3,4,5,6,7,8,9,10,11,12,13,14-dodecahydro-2H-cyclododeca[b]p	251-090-5	32539-83-6	32539836	2655	Reach_2662	2394	222	56.8	1.6E-01	1.0E+00	6.0E+05			1.1E-06	1.1E-07	3.5E-07				19%	-9.4	-9.2	-10.7
diethyl fluoromalonate	216-490-6	1599-67-3	1599673	2070	Reach_1698	2395	309	70.8	1.2E-02	4.7E-06	1.0E+11			1.1E-06	1.1E-07	3.5E-07				14%	-9.4	-9.2	-10.9
isopropyl laurate	233-560-1	10233-13-3	10233133	1339	Reach_2284	2396	242	23.3	5.1E-01	9.0E-02	1.5E+06			1.1E-06	1.1E-07	3.5E-07				22%	-9.4	-9.2	-11.7
4-{2-[2-(2-hydroxybenzylidene)hydrazino]-2-oxoethyl}-4-methy	700-714-9	1254469-57-2	1254469572	5643	Reach_4977	2397	314	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.9	-9.2	-10.8
isopropyl chloroformate	203-563-2	108-23-6	108236	1479	Reach_736	2398	123	-68.2	4.0E+03	4.4E+03	1.1E+01			1.1E-06	3.5E-07	1.1E-06				16%	-9.5	-9.2	-11.3
1,1'-(methylenedi-p-phenylene)bismaleimide	238-969-9	14901-07-6	14901076	477	Reach_2373	2399	192	52.5	3.0E+00	3.2E+02	2.6E+04		0	6.3E-08	3.5E-07	1.1E-06				14%	-8.2	-9.2	-11.1
4-chloro-α,α,α-trifluoro-3-nitrotoluene	204-451-6	121-17-5	121175	1723	Reach_1008	2400	226	52.1	1.6E+01	5.7E+01	2.6E+03			1.1E-06	3.5E-08	1.1E-07				16%	-9.4	-9.2	-11.1
3-methoxypropylamine	226-241-3	5332-73-0	5332730	3095	Reach_2097	2401	89	-40.4	2.3E+03	3.2E+05	3.8E-01		4.1	3.5E-06	3.5E-07	1.1E-06				14%	-9.4	-9.2	-10.9
tetramethyl orthosilicate	211-656-4	681-84-5	681845	3508	Reach_1497	2402	152	-41.7	2.0E+03	2.8E+04	1.2E-02			1.1E-06	3.5E-07	1.1E-06				15%	-9.4	-9.2	-10.8
N-(4-chloro-2,5-dimethoxyphenyl)-2-[[2,5-dimethoxy-4-[(phen	235-427-3	12225-18-2	12225182	1745	Reach_2305	2403	591	334.2	1.6E-16	3.9E-02	1.1E+04	8.56	14.9	1.1E-06	3.5E-08	1.1E-07				14%	-8.6	-9.2	-11.3
cholesterol	200-353-2	57-88-5	57885	3240	Reach_44	2404	387	162.1	2.4E-05	1.4E-03	5.5E+08	16		1.1E-06	1.1E-07	3.5E-07				23%	-8.9	-9.2	-10.0
6,15-dihydroanthrazine-5,9,14,18-tetrone	201-375-5	81-77-6	81776	940	Reach_277	2405	442	301.2	1.3E-16	8.1E-03	5.4E+07			3.0E-09	3.5E-07	1.1E-06				24%	-8.4	-9.2	-9.7
isobutyryl chloride	201-194-1	79-30-1	79301	3770	Reach_238	2406	107	-66.6	8.0E+03	6.6E+03	2.8E+00			1.1E-06	3.5E-07	1.1E-06				16%	-9.5	-9.2	-11.4
3,4-dimethoxyphenylacetonitrile	619-811-1	287930-71-6	287930716	5819	Reach_4547	2407	531	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				14%	-9.3	-9.2	-11.2
3,3'-[(2,5-dichloro-p-phenylene)bis[imino(1-acetyl-2-oxoethyle	219-292-8	2403-89-6	2403896	2369	Reach_1798	2408	171	43.7	8.5E-01	1.4E+04	1.4E+01	15.1	4.6	1.1E-06	1.1E-07	1.1E-06				23%	-9.1	-9.2	-10.1
heptanoyl chloride	219-775-3	2528-61-2	2528612	2428	Reach_1831	2409	149	-18.3	8.5E+02	1.5E+02	9.5E+01			3.5E-07	1.1E-07	3.5E-07				21%	-9.5	-9.2	-11.7
dodecanenitrile	219-440-1	2437-25-4	2437254	559	Reach_1810	2410	181	24.7	8.4E-01	6.4E+00	5.9E+04			6.0E-07	3.5E-08	1.1E-07				18%	-9.4	-9.2	-10.6
2,2-difluoro-1,3-benzodioxole	210-565-7	618-83-7	618837	3357	Reach_1439	2411	182	159.4	5.6E-07	7.6E+03	1.9E+01			3.5E-06	3.5E-07	1.1E-06				16%	-9.5	-9.2	-10.9
605-350-3	605-350-3	16397-70-9	16397709	2091	Reach_4172	2412	279	123.8	7.7E-04	2.2E+00	1.0E+05			1.1E-06	1.1E-07	3.5E-07				17%	-9.3	-9.2	-10.9
valeryl chloride	211-330-1	638-29-9	638299	3418	Reach_1477	2413	121	-42.4	4.0E+03	2.6E+03	1.0E+01			1.1E-06	3.5E-07	1.1E-06				17%	-9.5	-9.2	-11.5
decyldimethylamine	214-302-7	1120-24-7	1120247	1568	Reach_1656	2414	185	0.8	1.4E+01	1.7E+00	2.9E+04		3.9	3.5E-07	3.5E-08	1.1E-07				22%	-9.5	-9.2	-11.7
3'-chloropropiophenone	252-242-3	34841-35-5	34841355	2716	Reach_2683	2415	169	31.6	5.2E+00	4.1E+01	6.5E+02			3.5E-07	1.1E-07	3.5E-07				17%	-9.5	-9.2	-10.7
α,α,α',α'-tetramethyl-m-xylene-α,α'-diol	217-886-1	1999-85-5	1999855	2247	Reach_1742	2416	194	78.2	4.2E-03	8.8E+02	2.0E+02	14.5		1.1E-06	1.1E-07	3.5E-07				15%	-8.8	-9.2	-11.1
2-bromo-2-methylpropionyl bromide	213-339-6	938-18-1	938181	4085	Reach_1612	2417	183	54.3	1.4E+00	1.2E+02	1.2E+03			3.5E-07	3.5E-08	1.1E-07				17%	-9.5	-9.2	-11.5
Propanenitrile, 3-[[3-(tridecyloxy)propyl]amino]-, branched	203-810-4	110-87-2	110872	1532	Reach_834	2418	84	-71.9	1.0E+04	1.3E+04	1.6E+01		0	1.1E-06	1.1E-07	3.5E-07				15%	-9.1	-9.2	-11.2
cyclohexyl methacrylate	202-943-5	101-43-9	101439	1322	Reach_578	2419	168	-13.1	2.9E+01	7.1E+02	3.5E+03			3.5E-06	3.5E-07	1.1E-06				15%	-9.5	-9.2	-10.8
methyl 3-aminocrotonate	210-249-9	611-07-4	611074	3325	Reach_1418	2420	174	92.8	1.3E-01	7.8E+02	3.5E+02			3.5E-06	1.1E-07	3.5E-07				14%	-9.4	-9.2	-10.9
620-460-1	620-460-1	34494-24-1	34494241	2708	Reach_4570	2421	128	41.6	2.1E-01	1.0E+06	6.0E-02	14.9	6.82	1.1E-06	3.5E-07	1.1E-06				14%	-8.2	-9.2	-11.2
methylcyclohexane	203-624-3	108-87-2	108872	246	Reach_759	2422	98	-74.2	5.5E+03	2.7E+01	3.9E+03			2.1E-08	1.1E-07	3.5E-07				24%	-9.5	-9.2	-11.9
3-ethyloxetane-3-methanol	221-254-0	3047-32-3	3047323	2598	Reach_1904	2423	116	0.8	3.1E+01	1.3E+05	2.2E+00	15.5		1.1E-06	3.5E-07	1.1E-06				14%	-9.4	-9.2	-11.1
diethyl phosphonate	212-091-6	762-04-9	762049	3705	Reach_1534	2424	138	-27.6	9.3E+02	2.0E+05	7.1E-01			1.1E-06	3.5E-07	1.1E-06				14%	-9.4	-9.2	-10.8
606-753-7	620-464-3	1003859-14-0	1003859140	1303	Reach_4571	2425	207	46.1	3.9E+00	9.6E+03	8.5E+00		9.04	3.5E-07	3.5E-08	1.1E-07				14%	-8.2	-9.2	-11.3
methylurea	208-031-3	506-30-9	506309	3012	Reach_1310	2426	313	149.5	1.9E-02	2.2E-03	8.5E+08	4.9	0	1.1E-06	1.1E-07	3.5E-07				16%	-9.2	-9.2	-11.0
Salt of (8α,9R)-cinchonan-9-ol and [(R)-[(1S)-2-methyl-1-(1-oxo	204-118-5	115-96-8	115968	10	Reach_948	2427	285	83.0	5.2E-02	4.7E+02	4.3E+01									18%	-8.9	-9.2	-10.9
cyclohexapentylose	233-007-4	10016-20-3	10016203	1295	Reach_2277	2428	973	349.8	0.0E+00	1.0E+06	1.7E-08	11.8		1.1E-06	3.5E-07	1.1E-06				18%	-9.0	-9.2	-10.9
octadecylamine	204-695-3	124-30-1	124301	1791	Reach_1076	2429	270	94.3	1.2E-02	9.7E-04	5.1E+07		3.5	1.1E-06	1.1E-07	3.5E-07				23%	-9.2	-9.2	-11.5
2,2-Difluoroethanamine	278-077-7	75128-73-3	75128733	3658	Reach_2945	2430	309	287.5	3.2E-12	3.3E+04	1.8E-01		8.91	3.5E-06	3.5E-07	1.1E-06				14%	-9.4	-9.2	-10.7
3-methylpentane-1,5-diol	235-837-2	13001-46-2	13001462	5654	Reach_2315	2431	188	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-9.2	-9.2	-11.2
1,3-dihydro-1,3-dioxo-2H-isoindole-2-hexanoic acid	224-675-8	4443-26-9	4443269	2925	Reach_2037	2432	261	212.9	3.5E-08	2.5E+03	5.4E+02	4.86	14.5	3.5E-06	3.5E-07	1.1E-06				14%	-8.3	-9.2	-11.0
trichloro(ethyl)silane	204-072-6	115-21-9	115219	1633	Reach_940	2433	164	-64.1	4.9E+03	1.9E+04	3.2E+02			1.1E-06	3.5E-07	1.1E-06				15%	-9.5	-9.2	-11.1
2,4-dichloro-3-ethyl-6-aminophenol	214-406-2	1125-21-9	1125219	1591	Reach_1662	2434	152	56.0	2.5E+00	9.0E+03	7.6E+01	0	0	1.1E-06	3.5E-07	1.1E-06				14%	-8.6	-9.2	-11.3
thioacetamide	214-912-3	1210-35-1	1210351	1721	Reach_1674	2435	208	109.2	2.3E-02	5.7E+00	3.4E+04	0	0	3.5E-07	3.5E-08	1.1E-07				23%	-8.6	-9.2	-10.2
614-284-4	603-758-6	133647-88-8	133647888	5668	Reach_4128	2436	204	0.0												23%	-9.5	-9.2	-11.2
3-(4-tert-butylphenyl)propionaldehyde	242-016-2	18127-01-0	18127010	2166	Reach_2452	2437	190	46.3	6.7E-01	1.4E+02	8.7E+03			3.5E-07	3.5E-08	1.1E-07				17%	-9.5	-9.2	-10.7
3,9-dicyclohex-3-enyl-2,4,8,10-tetraoxaspiro[5.5]undecane	212-133-3	764-99-8	764998	3714	Reach_1538	2438	158	-17.9	7.6E+01	8.3E+03	1.7E+00			3.5E-07	1.1E-07	3.5E-07				16%	-9.0	-9.2	-11.0
1,2-dibromo-1,1,2,3,3,3-hexafluoropropane	210-513-3	617-45-8	617458	3351	Reach_1434	2439	133	218.2	3.5E-05	1.9E+05	4.8E-05			3.5E-06	3.5E-07	1.1E-06				23%	-9.5	-9.2	-11.9
3-(m-tert-butylphenyl)-2-methylpropionaldehyde	206-939-4	402-31-3	402313	2854	Reach_1266	2440	214	-45.9	2.5E+03	6.0E+01	8.3E+03			3.5E-07	3.5E-08	1.1E-07				18%	-9.5	-9.2	-10.7
4,4'-methylenedi-2,6-xylenol	226-378-9	5384-21-4	5384214	3112	Reach_2104	2441	256	162.0	2.6E-06	6.3E+00	1.7E+05	10.6		3.5E-07	3.5E-08	1.1E-07				19%	-8.7	-9.2	-10.8
butyronitrile	203-700-6	109-74-0	109740	1507	Reach_788	2442	69	-58.4	2.3E+03	4.5E+04	6.9E+00			3.5E-07	1.1E-07	3.5E-07				16%	-9.5	-9.2	-10.5
N,N-diethylhydroxylamine	223-055-4	3710-84-7	3710847	2791	Reach_1987	2443	89	7.8	4.6E+02	1.2E+05	2.7E+00		8.9	1.1E-05	3.5E-07	1.1E-06				14%	-8.9	-9.2	-11.2
3,4-dichloro-α,α,α-trifluorotoluene	248-885-4	28178-42-9	28178429	2524	Reach_2614	2444	203	21.4	3.3E+00	1.6E+01	3.2E+05			3.5E-07	3.5E-08	1.1E-07				23%	-9.5	-9.2	-11.9
2-bromopropane	203-558-5	108-18-9	108189	231	Reach_732	2445	101	-77.7	8.8E+01	6.0E+04	4.4E+01			5.0E-07	1.1E-07	3.5E-07				19%	-9.5	-9.2	-12.0
prasterone	200-175-5	53-43-0	53430	3101	Reach_20	2446	288	144.6	3.3E-06	3.6E+01	9.5E+02	16		3.5E-07	3.5E-08	1.1E-07				16%	-8.5	-9.2	-11.0
undecane	214-300-6	1120-21-4	1120214	1567	Reach_1655	2447	156	-32.4	8.4E+01	1.1E-01	5.5E+05			3.5E-07	3.5E-08	1.1E-07				23%	-9.5	-9.2	-12.0
2-methylbutyronitrile	700-143-5	959624-24-9	959624249	4139	Reach_4779	2448	256	154.6	1.8E-07	1.1E+02	1.2E+02			1.1E-06	3.5E-08	1.1E-07				17%	-9.5	-9.2	-10.7
trichloro(2,4,4-trimethylpentyl)silane	613-073-4	6271-80-3	6271803	3376	Reach_4379	2449	234	122.8	1.1E-03	2.1E+00	1.7E+04			1.1E-07	3.5E-08	3.5E-08				19%	-9.5	-9.2	-11.4
1,4-bis[(2,6-diethyl-4-methylphenyl)amino]anthraquinone	251-178-3	32724-62-2	32724622	2660	Reach_2665	2450	531	302.0	3.1E-14	9.6E-08	6.9E+12		14.4	1.1E-06	1.1E-07	3.5E-07				24%	-9.4	-9.2	-9.6
Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol	272-469-1	68855-18-5	68855185	3527	Reach_2910	2451	216	57.3	1.4E-02	2.3E+02	1.7E+03	15.3		3.5E-06	3.5E-07	1.1E-06				14%	-9.4	-9.2	-11.1
6-[[(4-methylphenyl)sulphonyl]amino]hexanoic acid	278-934-5	78521-39-8	78521398	3751	Reach_2954	2452	285	185.7	2.1E-06	3.2E+02	4.0E+02	4.88		3.5E-06	3.5E-07	1.1E-06				14%	-8.5	-9.2	-11.2

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Ethyl 1-[(2'-cyanobiphenyl-4-yl)methyl]-4-(2-hydroxypropan-2-	201-377-6	81-81-2	81812	942	Reach_278	2453	308	197.1	1.5E-09	4.0E+01	1.7E+02	4.86	0	4.5E-07	1.1E-07	3.5E-07				14%	-8.8	-9.2	-11.3
1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-8-iodooctane	606-722-8	211915-06-9	211915069	2286	Reach_4213	2454	628	349.8	4.2E-18	4.8E-03	3.8E+05			1.1E-06	1.1E-07	3.5E-07				23%	-9.4	-9.2	-11.9
1,3-dimethylimidazolidin-2-one	201-304-8	80-73-9	80739	3797	Reach_269	2455	114	18.4	1.7E+01	9.4E+04	4.9E-01		13.9	1.1E-06	1.1E-07	3.5E-07				14%	-9.4	-9.2	-11.3
methyl 4-[[(2,5-dichlorophenyl)amino]carbonyl]-2-[[2-hydroxy-	263-272-1	61847-48-1	61847481	3356	Reach_2852	2456	643	349.8	2.2E-22	3.2E-05	1.2E+08	9.4		3.5E-07	3.5E-08	1.1E-07				23%	-8.8	-9.2	-10.0
2-Chloro-2-methylpropanoyl chloride	202-188-1	92-77-3	92773	4049	Reach_392	2457	263	205.2	5.0E-09	1.1E+01	3.0E+04			3.5E-07	3.5E-08	1.1E-07				18%	-9.6	-9.2	-11.3
piperonal	204-409-7	120-57-0	120570	1715	Reach_998	2458	150	56.0	1.4E+00	6.2E+03	5.9E+01			1.1E-06	3.5E-07	1.1E-06				14%	-9.5	-9.2	-11.1
2,2-dimethyl-1,3-propanediyl dioctanoate	250-575-9	31335-74-7	31335747	2625	Reach_2654	2459	357	25.7	5.8E-03	5.3E-02	4.6E+07			1.1E-06	1.1E-07	3.5E-07				22%	-9.2	-9.2	-10.7
Dimethyl((2-oxocyclohexyl)methyl)ammonium chloride	617-143-5	80675-49-6	80675496	3796	Reach_4446	2460	386	241.6	4.3E-10	8.0E+00	9.8E+02									18%	-8.9	-9.2	-10.9
o-phenetidine	202-356-4	94-70-2	94702	4109	Reach_417	2461	137	39.6	9.1E+00	4.7E+03	4.5E+01		9.4	1.1E-06	1.1E-07	3.5E-07				14%	-8.7	-9.2	-11.2
allyl methacrylate	202-473-0	96-05-9	96059	1043	Reach_449	2462	126	-56.1	8.9E+02	2.6E+03	1.3E+02			7.2E-07	3.5E-07	1.1E-06				16%	-9.5	-9.2	-11.0
ethyl 2-bromobutyrate	208-574-6	533-68-6	533686	3099	Reach_1330	2463	195	-17.6	1.5E+02	1.8E+03	1.3E+02			3.5E-06	3.5E-07	1.1E-06				14%	-9.5	-9.2	-11.0
isobutyl acrylate	203-417-8	106-63-8	106638	198	Reach_675	2464	128	-57.4	1.2E+03	4.0E+03	1.3E+02			4.3E-07	3.5E-07	1.1E-06				17%	-9.5	-9.2	-10.9
2,2,4-trimethylpentane-1,3-diol	205-619-1	144-19-4	144194	1974	Reach_1194	2465	146	9.0	4.7E-01	2.1E+04	3.1E+01	15.3		3.5E-06	1.1E-06	3.5E-06				14%	-9.2	-9.2	-11.1
5-ethoxy-7-fluoro[1,2,4]triazolo[4,3-c]pyrimidine-3(2H)-thione	695-186-9	166524-68-1	166524681	2106	Reach_4688	2466	214	156.4	1.6E-04	4.1E+01	2.6E+01		15.1	1.1E-06	1.1E-07	3.5E-07				14%	-8.3	-9.2	-11.3
606-938-2	606-938-2	2212-11-5	2212115	1244	Reach_4226	2467	155	-45.0	9.9E+02	0.0E+00	6.9E+00			1.1E-06	3.5E-07	1.1E-06				14%	-9.5	-9.2	-10.8
methyl (R)-aminophenylacetate	204-594-4	123-04-6	123046	1760	Reach_1037	2468	149	-47.5	1.9E+02	1.4E+00	2.8E+04		0	3.5E-07	3.5E-08	1.1E-07				14%	-8.3	-9.2	-11.2
2,3-dichlorotoluene	256-636-6	50594-82-6	50594826	3011	Reach_2766	2469	249	25.0	2.5E+01	1.3E+00	7.8E+04			1.1E-07	1.1E-08	3.5E-08				21%	-9.5	-9.2	-11.1
(chloromethyl)triethoxysilane	239-311-3	15267-95-5	15267955	2025	Reach_2380	2470	213	7.6	1.7E+01	0.0E+00	1.1E+01			1.1E-06	3.5E-07	1.1E-06				14%	-9.5	-9.2	-11.2
methyl 2-amino-4-[[(2,5-dichlorophenyl)amino]carbonyl]benzo	261-853-4	59673-82-4	59673824	3283	Reach_2839	2471	339	216.3	2.1E-08	2.2E+00	1.8E+04	13.6	12.4	1.1E-06	3.5E-08	1.1E-07				14%	-8.7	-9.2	-11.3
1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone	208-806-6	542-18-7	542187	687	Reach_1346	2472	119	-57.2	7.7E+02	6.1E+02	2.3E+03		0	1.4E-08	1.1E-07	3.5E-07				14%	-8.3	-9.2	-11.4
1,2-dihydro-5-nitro-3H-1,2,4-triazol-3-one	213-254-4	932-64-9	932649	4066	Reach_1610	2473	130	161.2	7.8E-05	1.4E+05	1.9E-03			1.1E-06	1.1E-07	3.5E-07				14%	-8.1	-9.2	-11.4
3-chloropropyne	201-568-4	84-87-7	84877	3880	Reach_291	2474	224	173.0	1.3E-07	4.0E+03	3.4E-01			1.1E-06	1.1E-07	3.5E-07				22%	-9.7	-9.2	-11.5
acetone-dimethyl acetal	217-218-9	1779-49-3	1779493	5743	Reach_1719	2475	357	0.0												17%	-9.5	-9.2	-11.0
2,2-bis(bromomethyl)propane-1,3-diol	221-967-7	3296-90-0	3296900	2671	Reach_1943	2476	262	82.6	8.6E-04	2.9E+03	7.1E+00	14.1		3.5E-06	1.1E-06	3.5E-06				14%	-8.5	-9.2	-11.2
1-(dimethylamino)propan-2-ol	203-556-4	108-16-7	108167	1477	Reach_731	2477	103	-40.9	6.7E+02	8.2E+05	3.0E-01	15	5.2	3.5E-06	1.1E-06	3.5E-06				14%	-9.5	-9.3	-11.2
6-[methyl(phenylsulphonyl)amino]hexanoic acid, compound w	248-107-3	26919-50-6	26919506	5807	Reach_2596	2478	435	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.9	-9.3	-10.9
N-phenyl-N-[(trichloromethyl)thio]benzenesulphonamide	223-054-9	3710-30-3	3710303	2790	Reach_1986	2479	110	-71.2	3.0E+03	2.5E+01	1.0E+04			1.1E-06	1.1E-07	3.5E-07				16%	-9.0	-9.3	-11.1
N-[3-(dimethoxymethylsilyl)propyl]ethylenediamine	221-336-6	3069-29-2	3069292	2608	Reach_1909	2480	206	54.5	1.6E+00	7.5E+04	3.8E-01		4.28	3.5E-06	1.1E-06	3.5E-06				14%	-9.2	-9.3	-11.3
4-(2,6,6-trimethylcyclohex-1-ene-1-yl)-but-3-ene-2-one	219-110-7	2362-14-3	2362143	2353	Reach_1785	2481	296	180.9	1.7E-07	1.3E+00	1.3E+06			1.1E-06	1.1E-07	3.5E-07				21%	-9.5	-9.3	-10.5
N,N'-diacetylhydrazine	221-576-1	3148-73-0	3148730	2627	Reach_1921	2482	116	126.2	2.8E-03	4.8E+05	2.6E-02			1.1E-06	3.5E-07	1.1E-06				14%	-8.3	-9.3	-11.3
2-chloropropane	200-858-8	75-29-6	75296	3664	Reach_137	2483	79	-114.3	6.8E+04	4.3E+03	1.0E+02			3.5E-07	3.5E-08	1.1E-07				22%	-9.6	-9.3	-11.9
methyl 3-methyl-2-butenoate	937-695-3	1185167-55-8	1185167558	5618	Reach_5146	2484	243	0.0												14%	-9.5	-9.3	-10.9
29H,31H-phthalocyanine	237-335-9	13752-51-7	13752517	1911	Reach_2349	2485	248	124.3	1.1E-03	3.9E+04	1.4E-01		7.39	1.1E-06	1.1E-07	3.5E-07				23%	-9.0	-9.3	-10.0
α-bromotoluene	228-545-1	6291-85-6	6291856	3387	Reach_2162	2486	103	-28.0	1.0E+03	1.5E+05	1.2E+00			3.5E-07	1.1E-07	3.5E-07				17%	-9.5	-9.3	-10.9
618-990-3	618-990-3	939961-06-5	939961065	6087	Reach_4506	2487	322	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-8.9	-9.3	-10.9
phosgene	202-452-6	95-79-4	95794	4135	Reach_442	2488	142	41.8	6.1E+00	5.6E+02	1.9E+02			1.1E-06	3.5E-07	1.1E-06				23%	-9.8	-9.3	-11.9
ethyl 3-amino-1H-pyrazole-4-carboxylate	200-362-1	58-08-2	58082	66	Reach_45	2489	194	180.3	9.8E-07	3.2E+05	1.4E+00		0	6.8E-09	1.1E-07	3.5E-07				14%	-8.1	-9.3	-11.3
isodecyl methacrylate	249-978-2	29964-84-9	29964849	2581	Reach_2640	2490	226	13.7	1.6E+00	1.5E+00	4.2E+05			1.1E-06	1.1E-07	3.5E-07				20%	-9.5	-9.3	-11.4
1-(vinyloxy)octadecane	609-335-2	3717-40-6	3717406	2792	Reach_4297	2491	179	34.6	1.3E+01	4.4E+02	1.3E+03			3.5E-07	1.1E-07	3.5E-07				23%	-9.1	-9.3	-10.9
3,3'-[butane-1,4-diylbis(oxy)]bispropanamine	201-832-9	88-45-9	88459	3957	Reach_324	2492	188	161.3	6.6E-07	5.2E+04	2.8E-04		8.35	1.1E-06	1.1E-07	1.1E-06				14%	-8.3	-9.3	-11.4
octyltrichlorosilane	226-112-1	5283-66-9	5283669	678	Reach_2093	2493	248	8.1	9.4E+00	1.7E+02	2.8E+05			1.3E-07	1.1E-07	3.5E-07				21%	-9.5	-9.3	-10.6
2,4,6-tri-tert-butylphenol	211-989-5	732-26-3	732263	829	Reach_1524	2494	262	104.3	2.7E-02	2.6E-01	2.5E+06	12.1		2.2E-09	3.5E-07	1.1E-06				24%	-9.4	-9.3	-10.6
611-869-6	700-691-5	473799-16-5	473799165	2965	Reach_4969	2495	289	216.5	2.1E-08	1.8E+01	4.9E+00			1.1E-06	1.1E-07	3.5E-07				18%	-9.5	-9.3	-10.7
4-amino-6-chlorobenzene-1,3-disulphonamide	204-463-1	121-30-2	121302	1724	Reach_1009	2496	286	200.3	5.3E-08	4.7E+03	3.1E-01	7.8		3.5E-06	1.1E-07	3.5E-07				14%	-8.1	-9.3	-11.5
dodecane	203-967-9	112-40-3	112403	1587	Reach_904	2497	170	-20.9	3.1E+01	3.5E-02	1.7E+06			3.5E-07	3.5E-08	1.1E-07				23%	-9.5	-9.3	-12.0
2,4,6-trimethyl-2,4,6-tris(3,3,3-trifluoropropyl)cyclotrisiloxane	219-154-7	2374-14-3	2374143	2357	Reach_1790	2498	469	33.9	4.0E+01	1.8E-03	6.9E+09			3.5E-07	3.5E-08	1.1E-07				24%	-9.4	-9.3	-10.5
1-(allyloxy)-2-methyl-1-oxopropan-2-yl 2-chloro-5-[3-methyl-2,	603-837-5	134605-64-4	134605644	433	Reach_4131	2499	475	228.8	3.1E-09	2.6E-01	1.1E+03			9.9E-08	1.1E-07	3.5E-07				19%	-8.8	-9.3	-10.8
trans-crotonic acid	200-002-3	50-01-1	50011	2994	Reach_2	2500	59	18.4	2.9E+02	3.1E+05	2.3E-02	0		1.1E-06	3.5E-07	1.1E-06				14%	-8.4	-9.3	-11.2
chloroacetaldehyde	700-052-0	60046-50-6	60046506	3303	Reach_4741	2501	156	52.1	1.9E-01	2.0E+04	7.6E+00			1.1E-06	3.5E-07	1.1E-06				15%	-9.6	-9.3	-10.8
3,3'-sulphonyldianiline	209-967-5	599-61-1	599611	3298	Reach_1409	2502	248	182.9	4.1E-06	2.1E+03	5.9E+00		11	1.1E-06	3.5E-07	1.1E-06				14%	-8.3	-9.3	-11.2
4-tert-butylpyrocatechol	202-653-9	98-29-3	98293	4181	Reach_503	2503	166	83.3	4.4E-02	8.6E+02	8.7E+02	10		1.1E-05	1.1E-06	3.5E-06				14%	-9.4	-9.3	-11.1
1-nitropropane	203-544-9	108-03-2	108032	1475	Reach_726	2504	89	-26.2	1.3E+03	1.5E+04	8.9E+00	8.8		1.1E-05	1.1E-07	3.5E-07				14%	-9.5	-9.3	-11.2
5-propyl-1,3-benzodioxole	202-344-9	94-58-6	94586	4105	Reach_415	2505	164	43.5	7.4E+00	3.7E+01	3.8E+03			3.5E-07	3.5E-08	1.1E-07				18%	-9.6	-9.3	-10.8
bis(2-ethylhexyl) succinate	202-165-6	92-54-6	92546	4039	Reach_386	2506	162	70.6	2.1E-03	3.9E+03	3.5E+01			3.5E-07	1.1E-07	3.5E-07				21%	-9.3	-9.3	-10.7
2-methylbutan-1-ol	204-050-6	114-49-8	114498	5612	Reach_934	2507	384	0.0												14%	-9.5	-9.3	-10.9
6-[(1-oxomethyloctyl)amino]hexanoic acid	203-702-7	109-76-2	109762	265	Reach_790	2508	74	-11.3	8.5E+02	1.0E+06	7.4E-02	0	4	4.0E-07	1.1E-06	3.5E-06				16%	-8.5	-9.3	-11.1
4,4'-methylenedi-o-toluidine	223-342-4	3845-76-9	3845769	2822	Reach_1994	2509	156	82.0	9.4E-02	2.3E+04	7.1E-01		4.8	3.5E-06	3.5E-07	1.1E-06				14%	-8.7	-9.3	-11.3
bis(2-chloroethyl) 3,3'-[(2,5-dimethyl-p-phenylene)bis[iminocar	261-819-9	59587-44-9	59587449	3281	Reach_2838	2510	270	44.4	7.2E-02	1.4E-01	1.5E+07	0		1.1E-06	1.1E-07	3.5E-07				24%	-9.5	-9.3	-8.4
1,1-difluoroethane	200-866-1	75-37-6	75376	3669	Reach_142	2511	66	-158.1	5.1E+05	8.0E+03	1.3E+01			1.1E-06	3.5E-07	1.1E-06				20%	-9.6	-9.3	-12.0
11β,17,21-trihydroxypregna-1,4-diene-3,20-dione 21-methane	237-721-7	13940-94-8	13940948	1919	Reach_2352	2512	195	16.3	8.2E+00	1.5E+01	4.2E+03	0		1.1E-07	1.1E-08	3.5E-08				14%	-8.3	-9.3	-11.3
1-(2-hydroxyethyl)pyrrolidin-2-one	222-359-4	3445-11-2	3445112	1260	Reach_1962	2513	129	75.3	2.5E-02	2.4E+05	8.3E-02	14.9	14.7	3.5E-06	3.5E-07	3.5E-06				14%	-8.1	-9.3	-11.2
N,N-bis(3-aminopropyl)methylamine	277-873-1	74441-05-7	74441057	3635	Reach_2943	2514	499	349.8	4.5E-20	1.9E+01	4.6E+01		12	1.1E-06	3.5E-07	1.1E-06				14%	-9.0	-9.3	-11.4
dibutyl adipate	203-350-4	105-99-7	105997	184	Reach_653	2515	258	-6.6	3.6E-01	3.2E+01	2.1E+04			1.0E-06	3.5E-08	1.1E-07				16%	-9.5	-9.3	-10.8
619-636-0	265-633-9	65212-76-2	65212762	5972	Reach_2870	2516	551	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				14%	-8.6	-9.3	-11.2
5-chloro-α,α,α-trifluoro-2-nitrotoluene	610-840-5	52449-76-0	52449760	3059	Reach_4336	2517	206	117.9	4.0E-03	7.6E+01	1.5E+01			3.5E-06	3.5E-08	1.1E-07				15%	-9.5	-9.3	-10.8
4-methyl-3-decen-5-ol	279-815-0	81782-77-6	81782776	3814	Reach_2961	2518	170	-2.9	7.9E-01	2.1E+02	1.1E+04	15.5		1.1E-06	1.1E-07	3.5E-07				16%	-9.5	-9.3	-11.0
N,N''-(4-methyl-m-phenylene)bis[N',N'-dimethylurea]	241-523-6	17526-94-2	17526942	2141	Reach_2435	2519	264	193.0	7.1E-07	2.6E+03	5.9E+00	13.8	14.1	1.1E-06	1.1E-07	3.5E-07				14%	-8.2	-9.3	-11.4
617-707-0	618-771-2	915725-52-9	915725529	6081	Reach_4499	2520	186	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-8.3	-9.3	-11.3
allylamine	203-463-9	107-11-9	107119	209	Reach_694	2521	57	-73.1	3.4E+04	1.0E+06	1.6E+00		4	4.2E-07	3.5E-07	1.1E-06				16%	-9.5	-9.3	-10.5
(4-nonylphenoxy)acetic acid	221-486-2	3115-49-9	3115499	2619	Reach_1917	2522	278	146.1	1.3E-03	5.2E-02	6.3E+05	3.1		1.1E-06	3.5E-07	1.1E-06				14%	-8.8	-9.3	-11.3
2-[benzyl(2-hydroxyethyl)amino]-1-phenylethanol	203-994-6	112-64-1	112641	1596	Reach_917	2523	247	57.7	4.9E-01	6.4E-02	2.6E+05	0	0	1.1E-06	1.1E-07	3.5E-07				14%	-8.3	-9.3	-11.3
(R)-2,2,3-trimethylcyclopent-3-ene-1-acetaldehyde	224-815-8	4501-58-0	4501580	2937	Reach_2044	2524	152	11.5	3.2E+01	5.2E+02	2.0E+03			1.1E-06	3.5E-07	1.1E-06				15%	-9.6	-9.3	-10.7
2-methylbenzene-1,4-diyl bis{4-[4-(acryloyloxy)butoxy]benzoat	204-605-2	123-15-9	123159	385	Reach_1040	2525	100	-66.7	2.4E+03	6.3E+03	5.4E+01			8.9E-07	3.5E-07	1.1E-06				22%	-8.8	-9.3	-10.1
N-(2-hydroxypropyl)oleamide	203-828-2	111-05-7	111057	1537	Reach_843	2526	340	194.2	1.9E-09	2.5E-02	2.5E+06	13.7	14.7	1.1E-06	1.1E-07	3.5E-07				14%	-8.7	-9.3	-11.2
610-513-7	211-745-8	693-21-0	693210	804	Reach_1505	2527	196	29.1	3.9E+00	3.0E+04	7.9E+00	0	0	2.1E-06	1.1E-07	3.5E-07				14%	-8.5	-9.3	-11.2

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
alpha,2-dichloro-6-fluorotoluene	201-813-5	88-23-3	88233	3953	Reach_321	2528	224	173.7	2.3E-07	5.6E+03	1.2E-02			1.1E-06	1.1E-07	3.5E-07				18%	-9.6	-9.3	-11.0
cyclooctapentylose	241-482-4	17465-86-0	17465860	6398	Reach_2434	2529	1297	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.0	-9.3	-11.0
tetradecahydro-7-isopropyl-1,4a-dimethylphenanthren-1-meth	236-476-3	13393-93-6	13393936	1873	Reach_2333	2530	293	117.3	4.5E-05	2.1E-01	2.5E+06	15.9		3.5E-07	3.5E-08	1.1E-07				21%	-9.1	-9.3	-10.6
3,4-dimethoxyphenethylamine	614-070-0	674773-12-7	674773127	3492	Reach_4395	2531	254	129.1	4.0E-04	2.1E+03	8.3E+00		0	1.1E-06	1.1E-07	1.1E-06				14%	-9.5	-9.3	-11.3
N-(2-chlorobenzyl)-1-phenylpropan-2-amine hydrochloride (1::	695-069-2	1048649-80-4	1048649804	5594	Reach_4686	2532	296	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.0	-9.3	-11.0
1,1-dimethoxytrimethylamine	200-939-8	76-16-4	76164	3701	Reach_173	2533	138	-155.7	2.0E+06	5.2E+01	1.4E+02		0	3.5E-08	1.1E-08	3.5E-08				14%	-8.9	-9.3	-11.3
isobutyric anhydride	202-603-6	97-72-3	97723	4171	Reach_485	2534	158	-67.6	1.1E+02	3.5E+03	1.7E+01			3.5E-06	3.5E-07	1.1E-06				14%	-9.5	-9.3	-11.0
dichloro(chloromethyl)methylsilane	700-442-0	73573-88-3	73573883	3623	Reach_4900	2535	391	201.1	1.1E-09	6.5E+00	2.1E+04			1.1E-06	1.1E-07	3.5E-07				22%	-9.7	-9.3	-11.6
1,2,3,6-tetrahydro-3-methylphthalic anhydride	226-247-6	5333-84-6	5333846	3097	Reach_2099	2536	166	6.5	3.9E+00	4.9E+03	2.4E+02			3.5E-06	3.5E-07	1.1E-06				14%	-9.6	-9.3	-11.2
2,6-dimethylheptan-4-one	203-620-1	108-83-8	108838	1490	Reach_758	2537	142	-41.4	2.9E+02	1.1E+03	3.6E+02			1.1E-06	3.5E-07	1.1E-06				15%	-9.6	-9.3	-11.0
1,4-bis(mesitylamino)anthraquinone	204-155-7	116-75-6	116756	1653	Reach_956	2538	475	280.3	9.8E-13	3.8E-06	7.4E+10		14.4	1.1E-06	3.5E-07	1.1E-06				24%	-9.4	-9.3	-9.8
610-555-6	619-405-4	99199-60-7	99199607	4199	Reach_4518	2539	196	99.1	2.1E-02	3.4E+03	1.3E+02			1.1E-06	3.5E-07	1.1E-06				15%	-9.6	-9.3	-11.0
methyl 4-tert-butylbenzoate	225-756-0	5056-17-7	5056177	3009	Reach_2074	2540	164	6.5	1.4E+00	2.5E+03	5.5E+01			3.5E-06	3.5E-07	1.1E-06				16%	-9.6	-9.3	-10.8
1,2-epoxycyclohexane	206-007-7	286-20-4	286204	2539	Reach_1221	2541	98	-52.3	1.5E+03	2.0E+04	4.6E+01			1.1E-06	1.1E-07	3.5E-07				15%	-9.6	-9.3	-10.7
2,3-epoxypropan-1-ol	209-128-3	556-52-5	556525	703	Reach_1366	2542	74	-42.7	7.5E+02	1.6E+06	8.1E-02	15		1.3E-06	3.5E-07	1.1E-06				14%	-9.5	-9.3	-11.3
phenyl chloroformate	205-498-5	141-75-3	141753	1941	Reach_1167	2543	107	-54.8	5.3E+03	5.2E+03	3.2E+00			1.1E-06	3.5E-07	1.1E-06				15%	-9.6	-9.3	-10.9
dimethyl naphthalene-2,6-dicarboxylate	212-661-4	840-65-3	840653	3856	Reach_1565	2544	244	25.1	3.2E-02	3.2E+01	6.9E+02			1.1E-06	1.1E-07	3.5E-07				15%	-9.6	-9.3	-11.2
6-methyl-2-oxoperhydropyrimidin-4-ylurea	216-223-3	1530-32-1	1530321	2028	Reach_1689	2545	371	150.7	8.9E-06	5.3E-03	8.1E-01	0	0	1.1E-07	3.5E-09	1.1E-08				14%	-8.3	-9.3	-11.4
617-931-9	616-378-0	767340-03-4	767340034	3723	Reach_4436	2546	405	185.1	2.3E-06	1.6E+00	3.4E+01			1.1E-06	1.1E-07	3.5E-07				16%	-9.6	-9.3	-10.6
606-859-3	606-859-3	21890-10-8	21890108	2311	Reach_4221	2547	252	105.2	2.3E-03	3.1E+00	8.1E+03			1.1E-06	1.1E-07	3.5E-07				16%	-9.6	-9.3	-11.2
4,4'-[(6-chloro-1,3,5-triazine-2,4-diyl)diimino]bis[5-hydroxy-6-[	303-152-9	94158-79-9	94158799	6089	Reach_3007	2548	1467	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.0	-9.3	-11.0
octamethylenediamine	206-764-3	373-44-4	373444	2796	Reach_1259	2549	144	38.4	7.1E+00	3.9E+03	2.1E+01		3.2	1.1E-06	1.1E-07	3.5E-07				14%	-9.6	-9.3	-11.1
tartaric anhydride dibenzoate	604-481-3	14559-13-8	14559138	1987	Reach_4156	2550	170	45.8	3.2E+00	4.4E+02	5.5E+02	0		1.1E-06	1.1E-07	3.5E-07				14%	-8.1	-9.3	-11.3
3-(isotridecyloxy)propylamine	256-881-9	50977-10-1	50977101	3024	Reach_2768	2551	257	81.0	2.3E-02	3.6E-01	2.5E+05		4.1	3.5E-07	3.5E-08	1.1E-07				20%	-9.6	-9.3	-10.6
bis(trimethoxysilylpropyl)amine	280-084-5	82985-35-1	82985351	3839	Reach_2964	2552	342	98.1	1.0E-02	4.4E+03	6.0E-02		4.23	3.5E-06	3.5E-08	3.5E-07				14%	-8.6	-9.3	-11.6
2-(2-hexyloxyethoxy)ethanol	203-988-3	112-59-4	112594	1593	Reach_914	2553	190	40.5	2.3E-01	1.2E+05	1.9E+01	14.9		3.5E-06	3.5E-07	1.1E-06				14%	-8.7	-9.3	-11.3
4,7-dihydro-2-isopropyl-1,3-dioxepin	700-842-5	1192015-20-5	1192015205	5620	Reach_5007	2554	475	0.0												15%	-9.6	-9.3	-10.8
undecanedioic acid	230-279-6	7005-47-2	7005472	3555	Reach_2219	2555	117	-20.6	1.0E+02	3.7E+05	8.7E-01	15		3.5E-06	1.1E-06	3.5E-06				14%	-8.7	-9.3	-11.3
Tris[3-bromo-2,2-bis(bromomethyl)propyl] phosphate	606-254-4	19186-97-1	19186971	2226	Reach_4202	2556	1019	90.3	2.7E-06	4.2E-08	1.1E+08			3.5E-07	3.5E-08	3.5E-07				23%	-9.3	-9.3	-11.2
hexyl acetate	205-572-7	142-92-7	142927	466	Reach_1186	2557	144	-32.6	1.9E+02	9.4E+02	6.8E+02			9.2E-07	3.5E-07	1.1E-06				16%	-9.6	-9.3	-11.0
ethyl 2-bromo-2-methylpropionate	209-980-6	600-00-0	600000	3302	Reach_1411	2558	195	-11.3	2.9E+02	1.5E+03	1.2E+02			3.5E-06	3.5E-07	1.1E-06				14%	-9.6	-9.3	-11.3
7-[(E)-(4-aminophenyl)diazenyl]naphthalene-1,3,5-trisulfonic a	700-663-2	1035-69-4	1035694	1370	Reach_4962	2559	284	150.5	2.3E-04	1.4E+01	4.7E+02	0	0	3.5E-07	1.1E-07	3.5E-07				14%	-8.1	-9.3	-11.3
hexadecyl chloroformate	608-880-3	335153-21-4	335153214	2682	Reach_4284	2560	281	179.3	5.5E-06	2.2E+02	5.6E+02			1.1E-06	1.1E-07	1.1E-06				23%	-9.4	-9.3	-11.7
octadecyl isocyanate	204-019-7	112-96-9	112969	1614	Reach_932	2561	296	109.9	2.6E-01	5.8E-04	1.4E+09			1.1E-06	1.1E-07	3.5E-07				23%	-9.2	-9.3	-10.8
605-991-9	225-060-7	4635-87-4	4635874	2952	Reach_2051	2562	81	-46.7	5.4E+02	6.4E+03	1.3E+01			3.5E-07	1.1E-07	3.5E-07				14%	-8.9	-9.3	-11.3
chlorodimethylvinylsilane	217-007-1	1719-58-0	1719580	2125	Reach_1712	2563	121	-91.5	1.0E+04		6.9E+02			1.1E-06	1.1E-07	3.5E-07				20%	-9.6	-9.3	-12.2
ethyl vinyl ether	203-718-4	109-92-2	109922	1512	Reach_797	2564	72	-102.6	7.0E+04	7.2E+03	8.1E+00			1.1E-06	1.1E-07	3.5E-07				18%	-9.7	-9.3	-12.0
605-955-2	609-920-2	4137-56-8	4137568	2875	Reach_4316	2565	358	185.9	2.0E-06	2.0E+02	1.3E+01			3.5E-07	3.5E-08	1.1E-07				14%	-8.8	-9.3	-11.3
homosalate	204-260-8	118-56-9	118569	1673	Reach_965	2566	262	120.6	3.7E-04	6.9E+00	1.4E+06	9.8		1.1E-06	1.1E-07	3.5E-07				20%	-9.2	-9.3	-10.8
N-[3-(dimethylamino)propyl]-N,N',N'-trimethylpropane-1,3-dia	223-362-3	3855-32-1	3855321	2824	Reach_1996	2567	201	32.7	4.6E+00	4.7E+04	2.6E+00		4.17	3.5E-06	1.1E-07	3.5E-07				14%	-9.5	-9.3	-11.5
ethylene diformate	211-077-7	629-15-2	629152	3386	Reach_1465	2568	118	-102.5	1.7E+02	2.6E+05	2.0E-01			3.5E-06	3.5E-07	1.1E-06				14%	-9.5	-9.3	-11.3
2-benzoyl-1,2,3,6,7,11b-hexahydro-4H-pyrazino[2,1-a]isoquinc	600-478-6	1037197-98-0	1037197980	1379	Reach_4066	2569	335	160.5	3.6E-06	6.6E-02	2.0E+06		0	3.5E-07	3.5E-08	1.1E-07				20%	-8.7	-9.3	-10.7
vinyl laurate	620-166-3	32257-57-1	32257571	5843	Reach_4560	2570	1093	0.0												19%	-9.6	-9.3	-11.0
4-methyloxazole-5-carboxamide	700-281-6	2897-00-9	2897009	2553	Reach_4840	2571	286	146.3	9.3E-05	1.7E+00	3.3E+05	0	13	3.5E-08	1.1E-08	3.5E-08				14%	-8.1	-9.3	-11.3
2,3-dichlorobuta-1,3-diene	216-721-0	1653-19-6	1653196	2099	Reach_1704	2572	123	-88.7	6.2E+03	5.2E+02	1.0E+03			3.5E-07	3.5E-08	1.1E-07				22%	-9.7	-9.3	-11.9
800-884-5	800-884-5	1154308-86-7	1154308867	1636	Reach_5048	2573	201	119.1	7.6E-05	8.5E+02	3.8E+01	14.4	14.7	1.1E-06	3.5E-07	1.1E-06				14%	-8.5	-9.3	-11.3
(-)-pin-2(3)-ene	232-077-3	7785-26-4	7785264	887	Reach_2273	2574	136	-13.6	5.4E+02	2.8E+01	1.9E+04			9.7E-08	3.5E-08	1.1E-07				23%	-9.6	-9.3	-11.9
diisopropyl succinate	213-110-0	924-88-9	924889	4037	Reach_1595	2575	202	-70.6	4.1E+01	2.4E+03	1.7E+02			3.5E-06	3.5E-07	1.1E-06				14%	-9.6	-9.3	-11.0
decanal	203-957-4	112-31-2	112312	1581	Reach_897	2576	156	-8.1	3.1E+01	5.2E+01	5.8E+03			3.5E-07	3.5E-08	1.1E-07				19%	-9.6	-9.3	-11.2
1,2-bis(2-methoxyethoxy)ethane	228-506-9	6284-40-8	6284408	770	Reach_2160	2577	195	129.0	1.8E-06	1.0E+06	7.1E-04			3.4E-07	1.1E-06	3.5E-06				15%	-9.5	-9.3	-11.3
N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2-m	257-515-0	51920-12-8	51920128	3049	Reach_2776	2578	561	349.8	2.0E-21	1.5E-02	9.3E+05	9.21	15.7	1.1E-06	1.1E-07	3.5E-07				14%	-8.8	-9.3	-11.3
2-Chloro-1,1-difluoroethane	201-984-6	90-31-3	90313	3997	Reach_363	2579	209	124.2	1.8E-03	2.1E+04	1.6E+03			1.1E-06	1.1E-07	3.5E-07				23%	-9.9	-9.3	-12.0
N,N'-hexane-1,6-diylbis(hexahydro-2-oxo-1H-azepine-1-carbox	227-563-7	5888-87-9	5888879	3258	Reach_2141	2580	395	301.0	3.6E-14	1.9E+01	4.9E+03	14	13.6	1.1E-06	1.1E-07	3.5E-07				15%	-8.6	-9.3	-11.2
2-(Propylsulfanyl)pyrimidine-4,6(1H,5H)-dione	603-883-6	134931-01-4	134931014	1884	Reach_4132	2581	749	349.8	1.8E-26	1.1E-01	1.9E+02	11.8		3.5E-06	3.5E-07	1.1E-06				14%	-8.3	-9.3	-11.3
1,1'-methylenebis[4-fluorobenzene]	207-274-2	457-68-1	457681	2945	Reach_1281	2582	204	40.6	1.4E+00	8.3E-01	2.6E+04			1.1E-06	3.5E-08	1.1E-07				19%	-9.6	-9.3	-11.6
clioquinol	200-431-6	59-50-7	59507	737	Reach_51	2583	143	36.2	1.4E+00	1.1E+03	5.0E+02	9.6	0	3.7E-09	3.5E-07	1.1E-06				14%	-8.9	-9.4	-11.4
1,6-dibromohexane	211-067-2	629-03-8	629038	3384	Reach_1463	2584	244	7.9	7.4E+00	1.5E+01	9.3E+03			3.5E-07	1.1E-07	3.5E-07				19%	-9.6	-9.4	-11.3
1-(3,4-dimethoxybicyclo[4.2.0]octa-1,3,5-trien-7-yl)methanami	227-285-6	5763-44-0	5763440	3235	Reach_2134	2585	139	165.5	4.2E-05	9.1E+04	1.0E+00		0	3.5E-06	3.5E-07	3.5E-07				14%	-9.0	-9.4	-11.3
α,α,α-trifluoro-o-toluoyl chloride	206-233-6	312-94-7	312947	2624	Reach_1233	2586	209	18.1	3.6E+01	2.5E+02	2.5E+02			1.1E-06	1.1E-07	3.5E-07				15%	-9.6	-9.4	-11.1
1-[(2-chloro-4-nitrophenyl)azo]-2-naphthol	220-562-2	2814-77-9	2814779	2523	Reach_1872	2587	328	203.6	2.1E-08	2.3E+00	3.5E+06	8.66		3.5E-07	3.5E-08	1.1E-07				22%	-8.9	-9.4	-10.5
dibutyl fumarate	203-327-9	105-75-9	105759	182	Reach_649	2588	228	-28.2	7.1E-01	1.3E+02	1.4E+04			1.2E-06	3.5E-07	1.1E-06				16%	-9.6	-9.4	-11.0
octadecane	211-659-0	682-01-9	682019	3509	Reach_1498	2589	264	49.0	7.3E+00	1.7E+01	1.0E+02			1.1E-06	1.1E-07	3.5E-07				23%	-9.3	-9.4	-10.8
hexadecyltrimethoxysilane	240-464-3	16415-12-6	16415126	2092	Reach_2419	2590	347	100.5	2.0E-03	1.6E-01	4.9E+06			1.1E-06	1.1E-07	3.5E-07				21%	-9.4	-9.4	-10.7
dodecan-5-olide	700-306-0	383412-05-3	383412053	2821	Reach_4852	2591	193	-1.7	9.9E+00	1.2E+02	3.2E+03			3.5E-06	3.5E-07	1.1E-06				17%	-9.6	-9.4	-10.9
docosanamide	221-304-1	3061-75-4	3061754	2604	Reach_1908	2592	340	182.7	9.7E-07	2.4E-05	4.6E+08	15.1	14.3	1.1E-06	1.1E-07	3.5E-07				23%	-9.1	-9.4	-10.2
619-635-5	619-635-5	12567-73-6	12567736	5644	Reach_4533	2593	440	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.0	-9.4	-11.0
N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-2-[(4-nitrophenyl)a	249-955-7	29920-31-8	29920318	2579	Reach_2638	2594	453	287.8	3.0E-13	3.8E+01	7.6E+01	8.71	12.1	1.1E-06	1.1E-07	3.5E-07				14%	-8.6	-9.4	-11.5
6-(isononanoylamino)hexanoic acid, compound with 2,2',2''-nit	203-842-9	111-18-2	111182	1540	Reach_847	2595	172	0.0	3.0E+01	8.4E+04	5.0E+01	0	3.63	3.5E-07	1.1E-07	3.5E-07				16%	-8.6	-9.4	-11.2
2-nitro-p-anisidine	202-547-2	96-96-8	96968	4157	Reach_472	2596	168	96.8	2.2E-02	1.0E+03	1.3E+02		13	3.5E-06	1.1E-07	3.5E-07				14%	-8.6	-9.4	-11.4
O,O-diethyl hydrogen phosphorodithioate	247-571-4	26266-68-2	26266682	2459	Reach_2577	2597	126	-40.4	6.2E+01	1.1E+03	4.2E+02	0		1.1E-06	3.5E-07	1.1E-06				22%	-9.6	-9.4	-10.6
5-nitro-o-toluidine	255-419-3	41506-62-1	41506621	2879	Reach_2744	2598	320	261.0	1.6E-12	5.1E+00	3.8E+03		13.3	3.5E-07	3.5E-08	1.1E-07				23%	-8.9	-9.4	-10.3
2,5-diaminobenzenesulphonic acid	246-141-3	24304-50-5	24304505	2385	Reach_2544	2599	304	231.4	2.1E-09	1.2E+03	9.8E-01	10.4	13.1	3.5E-07	1.1E-07	3.5E-07				14%	-8.1	-9.4	-11.4
2,2'-(cyclohexylimino)bisethanol	224-809-5	4500-29-2	4500292	2936	Reach_2043	2600	187	82.0	7.4E-04	1.7E+05	5.9E+00	14.7	4.6	3.5E-06	1.1E-06	3.5E-06				14%	-8.5	-9.4	-11.3
ethyl 2-[3-cyano-4-(2-methylpropoxy)phenyl]-4-methyl-1,3-thia	206-055-9	298-06-6	298066	591	Reach_1226	2601	186	-59.9	7.8E+00	4.8E+02	1.7E+02		0	2.0E-08	1.1E-07	1.1E-06				14%	-8.9	-9.4	-11.3
610-147-8	604-200-4	14078-41-2	14078412	1930	Reach_4144	2602	358	199.2	7.7E-09	1.3E-01	6.0E+06		0	1.1E-06	1.1E-07	3.5E-07				14%	-8.3	-9.4	-11.3

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
619-914-1	694-989-1	41131-49-1	41131491	5876	Reach_4685	2603	620	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				14%	-8.3	-9.4	-11.3
cis-2-tert-butylcyclohexyl acetate	243-718-1	20298-69-5	20298695	2258	Reach_2492	2604	198	10.9	7.1E+00	4.3E-01	2.6E+04			3.5E-06	3.5E-07	1.1E-06				18%	-9.7	-9.4	-12.5
ethyl phenyl(2,4,6-trimethylbenzoyl)phosphinate	805-107-3	40758-65-4	40758654	2865	Reach_5059	2605	193	64.9	1.4E+00	4.8E+02	5.0E+02			1.1E-06	1.1E-07	3.5E-07				15%	-9.4	-9.4	-11.3
propane-1,2,3-triyl trisheptanoate	210-647-2	620-67-7	620677	3361	Reach_1441	2606	429	81.0	4.4E-05	2.6E-02	5.4E+07			1.1E-06	1.1E-07	3.5E-07				22%	-8.9	-9.4	-10.4
1-(2,3-Dichlorophenyl)piperazine hydrochloride	202-940-9	101-41-7	101417	1321	Reach_577	2607	150	-0.5	2.1E+01	3.9E+04	1.2E+02									18%	-9.1	-9.4	-11.0
1,4-dioxacyclohexadecane-5,16-dione	259-423-6	54982-83-1	54982831	3157	Reach_2804	2608	256	63.4	3.3E-04	1.4E-02	1.7E+04			1.1E-06	1.1E-07	3.5E-07				16%	-9.6	-9.4	-10.9
5-(2-chloroethyl)-4-methyl-1,3-thiazole hydrochloride (1:1)	247-501-2	26175-68-8	26175688	2456	Reach_2576	2609	269	147.3	1.6E-04	5.7E+02	2.6E+01									18%	-9.1	-9.4	-11.0
trichlorotrifluoroethane	614-284-4	68127-98-0	68127980	3506	Reach_4397	2610	261	28.3	3.3E+01	6.2E+01	1.9E+03			3.5E-08	3.5E-08	1.1E-07				23%	-9.9	-9.4	-12.1
Ethyl 2-methylbut-3-enoate	211-550-8	661-95-0	661950	3466	Reach_1492	2611	310	-37.8	6.3E+03	5.1E+01	8.5E+03			1.1E-07	3.5E-08	1.1E-07				14%	-9.6	-9.4	-11.3
2-ethoxyphenol	202-358-5	94-71-3	94713	4111	Reach_418	2612	138	36.3	8.4E+00	1.5E+04	6.8E+01	10		3.5E-06	3.5E-07	1.1E-06				14%	-9.6	-9.4	-11.3
N-isopropylhydroxylamine	214-244-2	1117-31-3	1117313	1555	Reach_1650	2613	174	-82.7	1.7E+02	1.5E+04	2.0E+01		0	3.5E-06	3.5E-07	1.1E-06				14%	-9.5	-9.4	-11.2
[3-(triethoxysilyl)propyl]urea	245-876-7	23779-32-0	23779320	2358	Reach_2534	2614	264	129.6	1.3E-03	3.7E+03	7.2E-01	14.1	14.1	1.1E-06	3.5E-07	1.1E-06				14%	-8.5	-9.4	-11.4
N-(1,4-dimethylpentyl)-N'-phenylbenzene-1,4-diamine	221-374-3	3081-01-4	3081014	1257	Reach_1912	2615	282	129.8	2.8E-04	3.2E-01	1.5E+05		9.4	3.5E-06	1.1E-07	3.5E-07				14%	-8.9	-9.4	-11.4
4-nitro-m-xylene	231-274-1	7474-78-4	7474784	3643	Reach_2254	2616	188	161.3	6.6E-07	5.2E+04	1.0E-03			1.1E-06	1.1E-07	1.1E-06				14%	-9.6	-9.4	-11.0
bromotrifluoromethane	200-887-6	75-63-8	75638	3678	Reach_154	2617	149	-108.9	1.2E+06	2.1E+02	3.9E+01			3.5E-07	3.5E-08	1.1E-07				22%	-9.7	-9.4	-12.2
diisobutyl hexahydrophthalate	275-069-5	70969-58-3	70969583	815	Reach_2924	2618	284	-4.7	1.7E-01	2.3E+00	8.1E+04			3.2E-07	1.1E-07	3.5E-07				19%	-9.6	-9.4	-10.8
600-198-4	222-646-4	3564-28-1	3564281	5856	Reach_1972	2619	528	0.0	0.0E+00	0.0E+00	0.0E+00		0	0.0E+00	0.0E+00	0.0E+00				14%	-8.9	-9.4	-11.4
p-aminobenzamide	608-301-4	2896-99-3	2896993	2552	Reach_4270	2620	288	149.7	1.0E-06	2.2E+01	1.9E+04	14.7	10.6	1.1E-08	3.5E-09	1.1E-08				14%	-8.4	-9.4	-11.3
607-929-6	700-516-2	93413-62-8	93413628	4069	Reach_4917	2621	263	140.1	9.1E-06	6.1E+03	5.2E+02			1.1E-05	1.1E-06	3.5E-06				14%	-9.2	-9.4	-11.3
3'-(trifluoromethyl)acetophenone	258-556-7	53445-37-7	53445377	3103	Reach_2793	2622	188	115.5	7.0E-03	1.1E+04	3.3E+01			3.5E-06	3.5E-07	1.1E-06				15%	-9.6	-9.4	-11.0
613-198-4	613-198-4	63302-43-2	63302432	3397	Reach_4384	2623	206	89.3	2.7E-02	5.2E+01	9.1E+02		7.7	1.1E-06	1.1E-07	1.1E-06				15%	-9.6	-9.4	-11.3
2',3-bis[[3-[3,5-di-tert-butyl-4-hydroxyphenyl]propionyl]]propi	251-156-3	32687-78-8	32687788	2659	Reach_2664	2624	553	325.5	1.4E-18	3.6E-05	6.2E+07	11.7		1.1E-06	1.1E-07	3.5E-07				22%	-8.8	-9.4	-10.3
3,5-diamino-2,4,6-triiodobenzoic acid	619-914-1	1116495-86-3	1116495863	1552	Reach_4554	2625	255	227.8	3.6E-09	1.5E+01	3.4E+00	14.5	11.6	1.1E-06	3.5E-07	1.1E-06				14%	-8.5	-9.4	-11.4
6-methyloct-5-en-2-one	213-382-0	941-69-5	941695	4098	Reach_1614	2626	173	150.6	5.3E-04	4.9E+03	7.6E+00			1.1E-06	3.5E-07	1.1E-06				15%	-9.7	-9.4	-10.9
616-390-6	616-390-6	76811-98-8	76811988	3724	Reach_4437	2627	500	338.7	9.4E-19	3.2E-02	3.9E+02	3.99	4.9	1.1E-06	1.1E-07	3.5E-07				14%	-8.6	-9.4	-11.4
801-014-7	801-014-7	179107-88-1	179107881	2157	Reach_5050	2628	206	45.4	5.0E-01	1.1E+01	1.3E+05			1.1E-06	3.5E-07	1.1E-06				18%	-9.6	-9.4	-10.9
1-[bis[3-(dimethylamino)propyl]amino]propan-2-ol	266-587-2	67151-63-7	67151637	3487	Reach_2885	2629	245	89.1	1.4E-03	4.5E+04	7.2E-01	15	4.15	3.5E-06	1.1E-07	3.5E-07				14%	-8.3	-9.4	-11.6
617-349-5	617-589-0	84592-32-5	84592325	6053	Reach_4468	2630	576	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				15%	-8.5	-9.4	-11.3
heptan-1-ol	203-897-9	111-70-6	111706	308	Reach_866	2631	116	-26.0	4.0E+01	1.5E+03	2.0E+02	15.9		3.9E-06	1.1E-06	3.5E-06				14%	-9.6	-9.4	-11.0
Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo	271-878-2	68610-86-6	68610866	3522	Reach_2909	2632	688	349.8	6.0E-21	1.1E-05	1.3E+07	8.45	13.5	3.5E-07	3.5E-08	3.5E-08				22%	-8.7	-9.4	-10.4
6-[(1S)-1,3-dihydroxy-1-(1-trityl-1H-imidazol-4-yl)propyl]-N-me	700-333-8	1021394-33-1	1021394331	1337	Reach_4865	2633	486	272.7	3.3E-12	1.2E-02	1.3E+05	0	13.5	3.5E-06	1.1E-07	3.5E-07				19%	-8.9	-9.4	-11.0
614-070-0	608-307-7	2901-13-5	2901135	2555	Reach_4271	2634	192	28.3	3.0E+00	1.1E+02	2.8E+03			1.1E-06	1.1E-07	3.5E-07				14%	-8.6	-9.4	-11.4
(Z)-[cyano(2,3-dichlorophenyl)methylene]carbazamidine	700-837-8	1093205-95-8	1093205958	1499	Reach_5005	2635	159	101.5	8.0E-04	2.3E+04	1.5E+00		14.7	3.5E-06	3.5E-07	1.1E-06				19%	-8.7	-9.4	-11.0
vinyl 2-ethylhexanoate	202-297-4	94-04-2	94042	4096	Reach_410	2636	170	-21.8	5.5E+01	2.0E+02	4.0E+03			3.5E-06	3.5E-07	1.1E-06				15%	-9.7	-9.4	-11.4
dodecamethylpentasiloxane	275-662-9	71604-74-5	71604745	3586	Reach_2928	2637	277	127.5	7.6E-04	1.5E+03	7.4E+00			1.1E-06	1.1E-07	3.5E-07				24%	-9.6	-9.4	-10.5
4-hydroxymethyl-1,3-dioxolan-2-one	213-235-0	931-40-8	931408	4060	Reach_1608	2638	118	52.1	4.8E-04	1.2E+06	4.1E-02	13.7		1.1E-06	3.5E-07	1.1E-06				14%	-8.3	-9.4	-11.5
o-(trifluoromethyl)benzaldehyde	209-840-4	594-42-3	594423	3276	Reach_1398	2639	186	-22.1	6.0E+02	1.2E+02	3.0E+03			1.1E-07	1.1E-08	3.5E-08				15%	-9.7	-9.4	-11.0
tert-butyl α,α-dimethylbenzyl peroxide	222-389-8	3457-61-2	3457612	2709	Reach_1965	2640	208	35.3	3.0E+00	5.6E+01	4.6E+04			3.5E-07	3.5E-08	1.1E-07				18%	-9.7	-9.4	-10.7
1,4-bis[(2-ethyl-6-methylphenyl)amino]anthraquinone	255-460-7	41611-76-1	41611761	2881	Reach_2745	2641	475	280.3	9.8E-13	5.4E-06	5.8E+10		14.4	1.1E-06	1.1E-07	3.5E-07				24%	-9.5	-9.4	-9.9
(5-ethyl-1,3-dioxan-5-yl)methyl acrylate	266-380-7	66492-51-1	66492511	3475	Reach_2882	2642	200	44.6	1.9E+00	2.9E+03	2.8E+01			3.5E-06	3.5E-07	1.1E-06				14%	-9.6	-9.4	-11.3
5,6-Di-tert-butyl-21-({tert-butyl[1-(diethoxyphosphoryl)-2,2-dir	629-671-3	1522-41-4	1522414	2022	Reach_4594	2643	148	-29.6	3.6E+02	2.2E+03	4.6E-01									18%	-9.1	-9.4	-11.1
bis(triphenylphosphine)nickel(II) chloride	700-562-3	909782-32-7	909782327	4009	Reach_4935	2644	313	215.0	2.6E-08	7.7E+01	1.6E+03									18%	-9.1	-9.4	-11.1
Benzoic acid, 2-hydroxy-5-sulfo-, compd. with [4S-(4α,4aα,5α,5	205-811-5	152-97-6	152976	2026	Reach_1209	2645	376	204.9	5.2E-10	5.4E+01	1.1E+02									18%	-9.1	-9.4	-11.1
617-385-1	238-154-8	14264-16-5	14264165	6395	Reach_2362	2646	690	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.1	-9.4	-11.1
2,4,4-trimethylpentan-2-aminium (3R,5S,6E)-7-{4-(4-fluorophe	700-704-4	923036-25-3	923036253	4031	Reach_4974	2647	370	233.8	1.4E-09	5.1E-01	2.9E+03									18%	-9.1	-9.4	-11.1
Adenosine 5'-(trihydrogen diphosphate), 2'-(dihydrogen phosp	246-129-8	24292-60-2	24292602	5790	Reach_2542	2648	787	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.1	-9.4	-11.1
[3-(dimethylamino)propyl](triphenyl)phosphonium bromide hy	923-250-0	156755-23-6	156755236	2050	Reach_5098	2649	303	145.5	4.2E-05	2.5E+00	9.5E+02									18%	-9.1	-9.4	-11.1
dichloro(methyl)(phenyl)silane	205-746-2	149-74-6	149746	2006	Reach_1202	2650	191	-6.5	3.5E+01	3.0E+02	6.9E+03			3.5E-07	3.5E-08	1.1E-07				18%	-9.7	-9.4	-10.9
calcium N2,N6-bis(3-carboxypropanoyl)lysine (1:1)	700-699-9	877397-65-4	877397654	3940	Reach_4972	2651	209	58.1	1.0E-01	5.2E+02	9.5E+02									18%	-9.1	-9.4	-11.1
N,N-Dibenzyl-N-[2-(3,4-dihydroxyphenyl)-2-oxoethyl]ammoniu	613-308-0	63659-15-4	63659154	3415	Reach_4385	2652	282	124.2	3.9E-04	3.1E-01	2.2E+05									18%	-9.1	-9.4	-11.1
2-({6-[(3R)-3-Aminopiperidin-1-yl]-3-methyl-2,4-dioxo-3,4-dihy	700-046-8	16004-15-2	16004152	2071	Reach_4738	2653	297	48.9	6.7E-01	1.6E+01	1.1E+04									18%	-9.1	-9.4	-11.1
4-methoxy-3,5-dimethylpyridine-2-methanol	289-258-5	86604-78-6	86604786	3908	Reach_2990	2654	167	73.7	1.6E-02	1.9E+04	1.1E+01	13.7	10.3	1.1E-06	1.1E-07	3.5E-07				14%	-8.5	-9.4	-11.4
618-311-0	692-179-2	161798-01-2	161798012	2081	Reach_4674	2655	291	186.6	3.2E-07	4.4E+01	4.4E+03									18%	-9.1	-9.4	-11.1
1-bromohexadecane	204-008-7	112-82-3	112823	1606	Reach_925	2656	305	66.2	7.6E-02	4.0E-04	3.5E+08			1.1E-06	1.1E-07	3.5E-07				23%	-9.3	-9.4	-11.2
4-chlorobutyryl chloride	214-093-2	1079-66-9	1079669	1474	Reach_1644	2657	221	55.8	1.1E-01	1.5E+00	1.0E+04			1.1E-06	1.1E-07	3.5E-07				22%	-9.8	-9.4	-11.3
pyruvaldehyde	201-164-8	78-98-8	78988	3763	Reach_221	2658	72	-54.2	1.6E+04	7.4E+06	3.2E-02			3.5E-06	1.1E-06	3.5E-06				14%	-9.6	-9.4	-11.2
4-(cyclohexylcarbonoimidoyl)-5-(hydroxymethyl)-2-methylpyri	700-068-8	103953-71-5	103953715	1381	Reach_4749	2659	235	161.1	1.6E-05	2.7E+02	2.9E+03	0	14.4	1.1E-06	1.1E-07	3.5E-07				14%	-8.6	-9.4	-11.3
3-[(dimethylamino)methyl]-9-methyl-1,2,3,9-tetrahydro-4H-car	216-613-3	1624-62-0	1624620	2084	Reach_1700	2660	284	141.2	2.2E-04	1.8E+00	9.8E+03									18%	-9.1	-9.4	-11.1
(3R,4R)-1-benzyl-N,4-dimethylpiperidin-3-amine dihydrochloric	700-215-6	165670-57-5	165670575	2101	Reach_4807	2661	264	165.5	4.2E-05	3.6E-01	2.0E+03									18%	-9.1	-9.4	-11.1
2-(1-hydroxycyclohexyl)-2-(4-methoxyphenyl)ethyl ammonium	618-311-0	898543-06-1	898543061	6078	Reach_4493	2662	328	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.1	-9.4	-11.1
N,N,N-tripropylprop-2-en-1-aminium dicyanoazanide	700-603-5	908145-87-9	908145879	4007	Reach_4949	2663	377	199.4	4.4E-08	1.7E+00	5.1E+02									18%	-9.1	-9.4	-11.1
p-(trifluoromethoxy)phenyl isocyanate	252-328-0	35037-73-1	35037731	2720	Reach_2685	2664	203	-4.0	9.6E+01	5.1E+01	4.4E+03			1.1E-06	1.1E-07	3.5E-07				18%	-9.7	-9.4	-11.8
(2,2,8-trimethyl-4H-[1,3]dioxino[4,5-c]pyridin-5-yl)methanol hy	240-722-5	16673-34-0	16673340	2109	Reach_2426	2665	369	239.2	6.2E-10	5.6E+01	3.2E+02									18%	-9.1	-9.4	-11.1
1,3-bis(allylamino)propan-2-ol dihydrochloride	605-530-1	16874-33-2	16874332	2114	Reach_4177	2666	116	33.5	1.8E+01	5.2E+04	1.3E+00									18%	-9.1	-9.4	-11.1
2-aminododecan-1-ol hydrochloride (1:1)	246-403-7	24683-26-9	24683269	2401	Reach_2553	2667	283	182.2	5.3E-08	5.1E+02	3.0E+00									18%	-9.1	-9.4	-11.1
606-318-1	628-731-6	17159-79-4	17159794	2123	Reach_4588	2668	170	34.8	2.6E+00	1.0E+04	1.2E+01									18%	-9.1	-9.4	-11.1
2-(1-hydroxy-1-phenylethyl)pyridinium chloride	242-005-2	18109-80-3	18109803	2165	Reach_2451	2669	307	114.6	6.5E-03	3.0E+01	2.5E+03									18%	-9.1	-9.4	-11.1
1-ethyl-3-methyl-1H-imidazolium methanesulfonate (1:1)	226-137-8	5292-53-5	5292535	3081	Reach_2095	2670	248	2.6	1.2E-01	6.0E+01	8.7E+02									18%	-9.1	-9.4	-11.1
(3-chloro-4-methoxyphenyl)methanaminium chloride	700-268-5	18143-33-4	18143334	2167	Reach_4831	2671	139	-63.1	2.9E+03	0.0E+00	1.3E+02									18%	-9.1	-9.4	-11.1
phenylephrine hydrochloride	202-993-8	101-97-3	101973	1332	Reach_586	2672	164	10.6	1.2E+01	1.1E+03	3.7E+02									18%	-9.1	-9.4	-11.1
2-(2-methoxy-phenoxy)ethylammonium chloride	245-371-1	22990-77-8	22990778	2342	Reach_2526	2673	114	28.7	4.1E+01	1.0E+06	1.3E+00									18%	-9.1	-9.4	-11.1
Sodium 4-fluorobenzenesulfinate	807-096-0	917805-85-7	917805857	6082	Reach_5082	2674	611	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.1	-9.4	-11.1
615-083-4	219-397-9	2431-50-7	2431507	2386	Reach_1807	2675	159	-52.5	4.2E+02	1.3E+03	1.3E+03	0		1.1E-07	1.1E-08	3.5E-08				14%	-8.6	-9.4	-11.4
2-butyloctan-1-ol	223-470-0	3913-02-8	3913028	1263	Reach_2001	2676	186	18.8	1.9E-01	3.6E+00	5.0E+04	15.9		1.1E-06	1.1E-07	3.5E-07				17%	-9.7	-9.4	-10.8
mesitylene	201-099-5	78-26-2	78262	3749	Reach_196	2677	132	21.3	3.2E-01	1.2E+04	1.4E+01			1.1E-06	3.5E-07	1.1E-06				24%	-9.7	-9.4	-11.6

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
1,1'-[[3-(dimethylamino)propyl]imino]bispropan-2-ol	619-573-9	855425-38-6	855425386	3892	Reach_4530	2678	193	47.8	4.1E-01	2.4E+00	9.1E+04	0	0	3.5E-07	3.5E-08	1.1E-07				14%	-8.4	-9.4	-11.6
613-147-6	200-638-1	66-84-2	66842	5984	Reach_79	2679	216	0.0												15%	-9.7	-9.4	-11.0
1,5-dihydro-3-isopropyl-8-methyl-[1,3]dioxepino[5,6-c]pyridin-	249-922-7	29878-91-9	29878919	2576	Reach_2634	2680	342	255.3	5.1E-11	1.0E-01	7.4E+05		0	1.1E-07	3.5E-09	1.1E-08				14%	-8.7	-9.4	-11.4
bumetrizole	223-445-4	3896-11-5	3896115	1262	Reach_1998	2681	316	189.3	2.1E-07	1.1E+00	3.5E+05	10.2	15.5	3.5E-06	3.5E-07	1.1E-06				14%	-8.7	-9.4	-11.3
phenylephrine	700-018-5	50892-62-1	50892621	3020	Reach_4726	2682	245	184.9	2.4E-06	4.6E+01	1.5E+03	15.1	11.6	3.5E-06	1.1E-07	3.5E-07				14%	-8.5	-9.4	-11.4
tert-butyl isocyanate	201-874-8	89-00-9	89009	3966	Reach_336	2683	167	141.2	7.9E-05	7.9E+03	7.6E-01			3.5E-06	3.5E-07	1.1E-06				15%	-9.7	-9.4	-10.9
2-[(2-methyl-1-oxoallyl)oxy]ethyl acetoacetate	211-560-2	665-66-7	665667	5981	Reach_1493	2684	188	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-9.6	-9.4	-11.4
methyl 4-methyl-3-{[4-(pyridin-3-yl)pyrimidin-2-yl]amino}benzc	939-899-8	1441670-89-8	1441670898	1973	Reach_5161	2685	542	267.6	7.3E-12	5.8E-06	1.3E+08		9.03	1.1E-06	1.1E-07	3.5E-07				15%	-8.8	-9.4	-11.3
nonan-1-ol	264-347-1	63589-25-3	63589253	3412	Reach_2861	2686	295	300.2	2.7E-17	7.2E+01	5.1E-01	-1.76		3.5E-06	1.1E-07	3.5E-07				14%	-9.7	-9.4	-11.1
N-[4-(acetylamino)phenyl]-4-[[5-(aminocarbonyl)-2-chloropher	243-737-5	20325-40-0	20325400	5767	Reach_2493	2687	317	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				16%	-9.1	-9.4	-11.3
3,7-dimethyloct-6-en-1-yn-3-ol	249-482-6	29171-20-8	29171208	2560	Reach_2628	2688	152	15.4	4.6E+00	5.2E+02	5.6E+02	13.6		1.1E-06	1.1E-07	3.5E-07				15%	-9.7	-9.4	-11.0
3-methoxybutyl acetate	224-644-9	4435-53-4	4435534	2923	Reach_2036	2689	146	-38.2	3.7E+02	1.0E+04	1.0E+01			3.5E-06	3.5E-07	1.1E-06				14%	-9.7	-9.4	-11.1
pentadecan-15-olide	203-354-6	106-02-5	106025	1425	Reach_654	2690	240	26.1	6.9E-03	8.7E-01	1.4E+06			1.1E-06	1.1E-07	3.5E-07				20%	-9.5	-9.4	-10.9
ethyl methacrylate	202-597-5	97-63-2	97632	4167	Reach_483	2691	114	-67.1	2.4E+03	1.1E+04	5.9E+01			3.5E-06	3.5E-07	1.1E-06				14%	-9.7	-9.4	-11.3
thiophene	689-247-9	95149-35-2	95149352	4121	Reach_4649	2692	286	119.2	5.7E-04	7.4E-01	2.3E+07			3.5E-07	3.5E-08	1.1E-07				23%	-9.8	-9.4	-11.7
L-serine	200-274-3	56-45-1	56451	3199	Reach_29	2693	105	218.0	4.0E-06	1.9E+05	3.5E-04	2.1	4.9	3.5E-06	1.1E-06	3.5E-06				14%	-8.2	-9.4	-11.4
2-methylvaleric acid	219-823-3	2544-13-0	2544130	5797	Reach_1834	2694	257	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				15%	-9.2	-9.4	-11.3
4-phenylbutenone	204-555-1	122-57-6	122576	1752	Reach_1031	2695	146	11.9	1.3E+00	4.9E+02	1.1E+02			1.1E-06	1.1E-07	3.5E-07				14%	-9.7	-9.4	-11.2
2-nitro-p-xylene	616-206-4	7529-16-0	7529160	3662	Reach_4426	2696	111	63.1	7.2E-01	7.7E+04	2.8E+00			1.1E-06	1.1E-07	3.5E-07				14%	-9.7	-9.4	-11.1
615-161-8	201-744-0	87-41-2	87412	3932	Reach_309	2697	134	31.0	1.5E-01	4.7E+03	5.1E+00			3.5E-06	3.5E-07	1.1E-06				20%	-9.7	-9.4	-11.5
decahydronaphthalene	203-874-3	111-48-8	111488	1549	Reach_859	2698	122	24.9	3.2E-02	1.5E+05	2.4E-01			3.5E-06	1.1E-06	3.5E-06				24%	-9.7	-9.4	-12.1
p-[(2-chloroethyl)ethylamino]benzaldehyde	220-150-2	2643-07-4	2643074	1253	Reach_1850	2699	212	76.6	4.1E-02	1.2E+02	1.3E+03		13.5	1.1E-06	3.5E-07	1.1E-06				14%	-8.9	-9.4	-11.4
tert-butyl peroxypivalate	213-147-2	927-07-1	927071	4046	Reach_1599	2700	174	-13.2	2.0E+02	2.2E+02	6.3E+02			1.1E-06	3.5E-07	1.1E-06				17%	-9.7	-9.4	-11.6
2,4-xylenol	203-635-3	108-98-5	108985	1491	Reach_766	2701	110	-31.9	2.2E+02	3.7E+02	4.9E+02	6.8		3.5E-07	3.5E-08	1.1E-07				16%	-9.7	-9.4	-10.9
3-methylbutanone	209-264-3	563-80-4	563804	712	Reach_1375	2702	86	-79.5	7.3E+03	2.2E+04	4.7E+00			5.5E-07	3.5E-07	1.1E-06				16%	-9.7	-9.4	-11.1
1-(tetrahydrofuran-3-yl)methanamine	255-235-3	41131-65-1	41131651	2870	Reach_2736	2703	325	234.8	1.2E-09	6.1E+02	1.2E+00		14.5	3.5E-07	1.1E-07	3.5E-07				14%	-9.7	-9.4	-11.1
2-Propylheptan-1-amine	620-520-7	194608-78-1	194608781	2234	Reach_4575	2704	157	2.3	3.4E+01	3.3E+01	5.1E+03		3.5	3.5E-07	3.5E-08	1.1E-07				20%	-9.7	-9.4	-11.4
bisdecanoyl peroxide	212-092-1	762-12-9	762129	3706	Reach_1535	2705	343	14.3	5.9E-03	1.3E-02	2.4E+08			1.1E-06	1.1E-07	3.5E-07				23%	-9.3	-9.4	-10.9
cyclopropanecarbonyl chloride	689-242-1	95149-34-1	95149341	4120	Reach_4648	2706	272	110.2	1.3E-03	1.8E+00	7.4E+06			1.1E-06	1.1E-07	3.5E-07				15%	-9.7	-9.4	-11.1
triethylammonium bromide	211-263-8	636-70-4	636704	5963	Reach_1475	2707	182	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.1	-9.4	-11.1
2,6-di-tert-butyl-α-dimethylamino-p-cresol	201-816-1	88-27-7	88277	3954	Reach_322	2708	263	114.4	2.3E-03	9.0E+00	1.7E+04	11.6	5.06	1.1E-06	1.1E-07	3.5E-07				16%	-9.7	-9.4	-11.3
2-Chloro-3-(2,2,2-trifluoroethoxy)pyridine.	608-497-1	3056-13-1	3056131	2603	Reach_4276	2709	479	304.7	2.0E-14	1.3E-02	7.9E+03			1.1E-06	1.1E-07	3.5E-07				15%	-9.7	-9.4	-11.3
tetraethylammonium heptadecafluorooctanesulphonate	609-106-7	35249-89-9	35249899	5855	Reach_4289	2710	93	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.1	-9.4	-11.1
penta-1,3-diene	207-995-2	504-60-9	504609	3006	Reach_1305	2711	68	-108.6	5.5E+04	4.6E+02	2.8E+02			1.1E-06	1.1E-07	3.5E-07				20%	-9.8	-9.4	-12.4
1-[[(6R,7R)-7-amino-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]	700-425-8	521284-22-0	521284220	3053	Reach_4898	2712	256	157.1	4.2E-07	5.5E+03	2.1E+01									18%	-9.1	-9.4	-11.1
607-985-1	613-004-8	62285-89-6	62285896	5955	Reach_4378	2713	467	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				15%	-8.6	-9.4	-11.3
trichloromethanesulphenyl chloride	700-054-1	70905-68-9	70905689	3574	Reach_4742	2714	252	148.7	7.0E-07	3.5E+02	2.3E+02			3.5E-06	1.1E-06	3.5E-06				23%	-9.8	-9.4	-11.9
4-acetyl-1-methylpyridinium 4-methylbenzenesulfonate	298-613-3	93820-33-8	93820338	4086	Reach_2998	2715	269	130.0	2.7E-04	3.8E-02	1.1E+06									18%	-9.1	-9.4	-11.1
O-isopropyl ethylthiocarbamate	205-517-7	141-98-0	141980	460	Reach_1171	2716	147	12.9	4.9E+01	1.7E+03	8.5E+01	12		4.0E-09	3.5E-07	1.1E-06				23%	-9.7	-9.4	-10.7
lithium 3-[(3,4-dicyanophenyl)sulfanyl]propane-1-sulfonate.	606-216-7	190651-18-4	190651184	5753	Reach_4198	2717	437	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.1	-9.4	-11.1
2-[(3-aminopyrazolo[1,5-a]pyridin-2-yl)oxy]ethanol hydrochlor	254-235-0	38982-12-6	38982126	2830	Reach_2721	2718	232	132.4	1.2E-04	6.8E+00	1.5E+04									18%	-9.1	-9.4	-11.1
Trisodium [carboxy(oxido)methyl]phosphonate	695-745-7	1079221-49-0	1079221490	5604	Reach_4695	2719	231	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.1	-9.5	-11.1
2,6-dimethylcyclohexylamine	700-167-6	94695-50-8	94695508	4108	Reach_4787	2720	264	66.4	5.3E-01	1.1E+02	3.2E+02			3.5E-06	3.5E-07	1.1E-06				21%	-9.8	-9.5	-11.7
dimethyl [3-chloro-5-(trifluoromethyl)pyridin-2-yl]({[2-(trifluor	247-628-3	26351-32-6	26351326	2466	Reach_2580	2721	321	148.1	2.3E-05	1.5E-04	3.0E+07	0		1.1E-06	1.1E-07	3.5E-07				19%	-8.8	-9.5	-11.1
chloro(3-chloropropyl)dimethylsilane	700-310-2	71839-12-8	71839128	3592	Reach_4854	2722	207	73.1	1.0E-01	1.7E+02	2.1E+03			1.1E-06	1.1E-07	3.5E-07				23%	-9.8	-9.5	-11.8
2-phenylisobutyric acid	201-497-9	83-73-8	83738	3850	Reach_284	2723	397	154.2	3.3E-06	5.4E+00	1.0E+04	7.7		3.5E-07	3.5E-08	1.1E-07				14%	-8.7	-9.5	-11.5
2,2-dimethylbutyryl chloride	227-478-5	5856-77-9	5856779	3250	Reach_2138	2724	135	-35.5	1.5E+03	3.1E+03	2.4E+01			1.1E-06	3.5E-07	1.1E-06				15%	-9.7	-9.5	-11.4
etilefrine	206-490-4	349-76-8	349768	2719	Reach_1241	2725	188	5.9	5.1E+01	5.0E+02	4.4E+02			1.1E-06	1.1E-07	3.5E-07				14%	-8.6	-9.5	-11.4
Ammonium glycolate	619-072-5	94744-50-0	94744500	4113	Reach_4510	2726	325	199.9	2.5E-07	1.3E-01	2.5E+03									18%	-9.2	-9.5	-11.1
DL-lysine	212-201-2	768-94-5	768945	878	Reach_1543	2727	151	35.1	5.3E-01	6.8E+02	2.7E+02	0	4	1.7E-07	3.5E-07	1.1E-06				14%	-8.1	-9.5	-11.5
3,4-dimethoxy-N-methylphenethylamine	262-828-0	61516-73-2	61516732	3337	Reach_2850	2728	171	79.7	1.1E-01	5.3E+04	2.7E+00		15.8	3.5E-06	3.5E-07	1.1E-06				14%	-9.7	-9.5	-11.4
citraconic anhydride	210-459-0	616-02-4	616024	3341	Reach_1429	2729	112	-34.0	2.4E+01	5.4E+04	1.5E+02			3.5E-06	3.5E-07	1.1E-06				14%	-9.7	-9.5	-11.3
veratrole	202-045-3	91-16-7	91167	4013	Reach_370	2730	138	-5.6	3.6E+01	2.7E+03	4.4E+01			1.1E-06	3.5E-07	1.1E-06				14%	-9.7	-9.5	-10.9
3-(trifluoromethyl)benzoyl fluoride	226-518-9	5417-35-6	5417356	3130	Reach_2107	2731	142	-30.3	2.0E+02	3.0E+03	6.2E+01			1.1E-06	3.5E-07	1.1E-06				15%	-9.7	-9.5	-11.3
butane-1,4-disulfonic acid	269-507-4	68259-05-2	68259052	3513	Reach_2903	2732	926	349.8	1.1E-34	6.2E-12	6.5E+14	9.19		3.5E-07	1.1E-08	3.5E-08				14%	-8.2	-9.5	-11.6
cyclohexylethylcarbamoyl chloride	263-753-6	62899-75-6	62899756	3383	Reach_2855	2733	190	57.7	5.4E-01	3.2E+03	1.1E+02		14.4	1.1E-06	3.5E-07	1.1E-06				14%	-9.7	-9.5	-11.3
decamethyltetrasiloxane	204-606-8	123-17-1	123171	1764	Reach_1041	2734	186	-14.8	2.1E+00	9.4E+00	3.0E+04			1.1E-06	1.1E-07	3.5E-07				24%	-9.7	-9.5	-11.2
609-335-2	600-024-7	1000777-61-6	1000777616	5589	Reach_4054	2735	485	0.0	0.0E+00	0.0E+00	0.0E+00		0	0.0E+00	0.0E+00	0.0E+00				17%	-9.7	-9.5	-10.8
2-methylbut-3-en-2-ol	204-068-4	115-18-4	115184	1632	Reach_938	2736	86	-62.4	3.1E+03	1.1E+05	1.2E+01	15.5		3.5E-06	1.1E-06	3.5E-06				14%	-9.7	-9.5	-11.0
Tetrahydropyran-4-carboxaldehyde	700-032-1	50675-18-8	50675188	3015	Reach_4732	2737	114	-27.1	2.1E+02	2.8E+05	2.3E+00			1.1E-06	1.1E-07	3.5E-07				14%	-9.7	-9.5	-11.4
bis(2-ethylhexyl)amine	203-372-4	106-20-7	106207	1430	Reach_657	2738	241	28.2	7.1E-01	1.7E-03	3.6E+06		3.1	3.5E-07	3.5E-08	1.1E-07				23%	-9.7	-9.5	-12.2
[4-[4,4'-bis(dimethylamino)benzhydrylidene]cyclohexa-2,5-dier	208-953-6	548-62-9	548629	1220	Reach_1356	2739	408	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.1	-9.5	-11.1
2-(4-bromophenyl)-2-methylpropanoic acid	212-556-3	826-55-1	826551	3835	Reach_1557	2740	164	73.9	2.2E-01	4.2E+02	2.0E+02	4.3		1.1E-06	1.1E-07	3.5E-07				14%	-8.9	-9.5	-11.5
o-fluoro-α,α,α-trichlorotoluene	700-273-2	39627-98-0	39627980	2844	Reach_4833	2741	226	166.8	2.6E-05	7.0E+01	1.3E+02			3.5E-07	3.5E-08	1.1E-07				21%	-9.8	-9.5	-11.6
bromochloromethane	200-826-3	74-97-5	74975	844	Reach_120	2742	129	-70.5	1.9E+04	1.3E+04	2.7E+01			2.0E-08	3.5E-08	1.1E-07				23%	-9.8	-9.5	-11.6
dimethyl(octyl)amine	230-939-3	7378-99-6	7378996	833	Reach_2242	2743	157	-21.9	7.5E+01	3.0E+01	3.0E+03		4	1.0E-07	1.1E-07	3.5E-07				23%	-9.8	-9.5	-11.6
3-diethylaminopropiononitrile	617-349-5	82543-17-7	82543177	3830	Reach_4456	2744	387	216.9	1.2E-11	5.9E-01	1.6E+02		0	1.1E-06	1.1E-07	3.5E-07				14%	-9.7	-9.5	-11.3
α,α,α-trifluoro-o-toluidine	201-806-7	88-17-5	88175	3949	Reach_317	2745	161	9.6	6.7E+01	4.4E+03	1.1E+02		9.4	1.1E-06	3.5E-07	1.1E-06				14%	-9.6	-9.5	-11.4
octane	201-873-2	88-99-3	88993	990	Reach_335	2746	166	126.6	1.0E-04	2.8E+03	1.2E+01			1.1E-06	3.5E-07	1.1E-06				23%	-9.8	-9.5	-12.3
1-bromo-4-fluorobenzene	612-012-9	60728-43-0	60728430	3315	Reach_4370	2747	690	349.8	2.4E-22	6.0E-04	1.3E+05			3.5E-08	1.1E-08	3.5E-08				21%	-9.8	-9.5	-11.8
2-chlorobutane	201-151-7	78-86-4	78864	3760	Reach_212	2748	93	-101.1	1.9E+04	5.4E+02	3.1E+02			3.5E-07	3.5E-08	3.5E-07				22%	-9.8	-9.5	-12.2
1,2,3-Trichloro-5-(trichloromethyl)benzene	291-751-5	90474-13-8	90474138	4000	Reach_2994	2749	214	-34.2	4.6E+00	2.3E+03	4.0E+02			3.5E-06	3.5E-07	1.1E-06				23%	-9.7	-9.5	-11.6
thiodi(acetic acid)	204-663-9	123-93-3	123933	1777	Reach_1062	2750	150	110.1	7.3E-03	3.0E+04	6.9E-02	3.3		3.5E-06	3.5E-07	1.1E-06				14%	-8.3	-9.5	-11.5
2,2-dimethylpropane-1,3-diyl 2-ethylhexanoate	249-060-1	28510-23-8	28510238	2534	Reach_2619	2751	357	-0.7	1.3E-02	2.6E-03	3.2E+07			3.5E-07	3.5E-08	1.1E-07				23%	-9.6	-9.5	-11.6
p-cymene	202-796-7	99-87-6	99876	1092	Reach_540	2752	134	-28.2	1.5E+02	4.1E+01	1.0E+04			5.8E-07	3.5E-08	1.1E-07				20%	-9.8	-9.5	-11.8

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
615-275-8	617-834-1	863329-69-5	863329695	3904	Reach_4474	2753	479	198.8	3.0E-07	4.2E-02	8.3E+04	0		1.1E-06	1.1E-07	3.5E-07				14%	-9.5	-9.5	-11.4
propiophenone	202-257-6	93-55-0	93550	4072	Reach_402	2754	134	1.6	2.0E+01	7.7E+02	1.4E+02			3.5E-07	1.1E-07	3.5E-07				16%	-9.7	-9.5	-10.8
2-butylaminoethanol	201-089-0	78-16-0	78160	3748	Reach_195	2755	471	129.8	2.4E-06	3.0E-03	1.5E+09	0	0	1.1E-06	1.1E-07	3.5E-07				14%	-9.4	-9.5	-11.4
1,2,4-triazolo[4,3-a]pyridin-3(2H)-one	241-866-1	17927-72-9	17927729	5744	Reach_2447	2756	368	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				14%	-8.6	-9.5	-11.5
N,N-bis[3-(dimethylamino)propyl]-N',N'-dimethylpropane-1,3-c	251-459-0	33329-35-0	33329350	2680	Reach_2668	2757	272	87.2	2.3E-02	1.1E+04	4.0E+00		3.98	3.5E-06	1.1E-07	3.5E-07				14%	-8.7	-9.5	-11.7
dimethyl 5-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amin	244-815-1	22174-70-5	22174705	2322	Reach_2518	2758	272	33.2	3.1E-01	3.5E+00	3.4E+06	0	0	3.5E-07	3.5E-08	1.1E-07				14%	-8.6	-9.5	-11.5
619-015-4	619-015-4	943516-53-8	943516538	4101	Reach_4507	2759	229	174.8	1.1E-05	1.4E+03	1.5E+02		14.8	3.5E-07	1.1E-07	3.5E-07				16%	-8.8	-9.5	-11.3
(2S)-2-Benzyl-N,N-dimethylaziridine-1-sulfonamide	700-257-5	31251-41-9	31251419	2622	Reach_4826	2760	244	132.1	5.6E-04	1.5E+00	9.8E+03			1.1E-06	3.5E-08	1.1E-07				16%	-8.7	-9.5	-11.4
oxydiethylene dinitrate	212-603-8	831-52-7	831527	6046	Reach_1560	2761	221	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				14%	-9.7	-9.5	-11.5
2-ethylhexyl (3-isocyanatomethylphenyl)-carbamate	208-066-4	507-20-0	507200	3017	Reach_1316	2762	93	-99.5	3.9E+04	1.1E+03	2.8E+02	0		3.5E-07	1.1E-07	3.5E-07				19%	-9.5	-9.5	-11.1
ethylene diacetoacetate	200-306-6	57-00-1	57001	3220	Reach_35	2763	131	92.8	1.5E-03	1.5E+03	1.9E-04	2.6		3.5E-06	3.5E-07	1.1E-06				14%	-9.3	-9.5	-11.7
cyclohexylidenebis[tert-butyl] peroxide	221-111-2	3006-86-8	3006868	2584	Reach_1896	2764	260	65.7	5.9E-01	2.1E+01	1.9E+06			3.5E-07	3.5E-08	1.1E-07				21%	-9.7	-9.5	-10.7
m-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	205-492-2	141-63-9	141639	1940	Reach_1166	2765	385	-26.3	9.4E+00	8.5E-04	4.1E+09		0	3.5E-09	3.5E-09	3.5E-09				14%	-8.5	-9.5	-11.5
7-aminonaphthalene-1,3,5-trisulphonic acid	248-394-5	27310-25-4	27310254	2500	Reach_2600	2766	383	307.2	2.3E-19	2.9E-01	1.6E-03	-2.17	11.7	1.1E-06	1.1E-07	1.1E-06				14%	-8.2	-9.5	-11.5
butyryl chloride	217-547-8	1885-14-9	1885149	2212	Reach_1731	2767	157	0.4	1.0E+02	1.1E+03	2.2E+01			1.1E-06	3.5E-07	1.1E-06				16%	-9.8	-9.5	-11.6
2-(m-benzoylphenyl)propionitrile	225-302-1	4763-40-0	4763400	2968	Reach_2062	2768	238	95.4	4.9E-03	1.3E+00	5.5E+04			1.1E-06	1.1E-07	3.5E-07				15%	-9.6	-9.5	-11.4
p-tert-butylcinnamaldehyde	282-823-7	84434-23-1	84434231	3865	Reach_2975	2769	188	45.2	5.3E-01	1.1E+01	5.4E+03			3.5E-07	1.1E-07	3.5E-07				17%	-9.8	-9.5	-10.8
methyl 2-chloropropionate	241-624-5	17639-93-9	17639939	2147	Reach_2440	2770	123	-63.8	1.2E+03	1.2E+04	1.1E+01			3.5E-06	3.5E-07	1.1E-06				14%	-9.7	-9.5	-11.2
2,6,6-trimethylcyclohex-2-ene-1,4-dione	240-734-0	16690-93-0	16690930	5736	Reach_2427	2771	111	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				14%	-9.7	-9.5	-11.4
α,α,α-trifluoro-3-tolyl isocyanate	206-341-3	329-01-1	329011	2668	Reach_1237	2772	187	-21.5	2.8E+02	1.2E+03	3.6E+03			3.5E-06	1.1E-06	3.5E-06				15%	-9.8	-9.5	-11.5
dibutyl ether	205-575-3	142-96-1	142961	467	Reach_1187	2773	130	-50.4	1.0E+03	4.2E+02	1.0E+03			3.1E-08	1.1E-07	3.5E-07				23%	-9.8	-9.5	-11.6
methyl cholate	215-903-7	1448-36-8	1448368	1982	Reach_1681	2774	423	218.0	9.4E-12	5.1E+01	6.3E+03	15.4		1.1E-06	1.1E-07	3.5E-07				15%	-8.7	-9.5	-11.3
[[(phosphonomethyl)imino]bis[ethylenenitrilobis(methylene)]]t	700-525-1	54090-39-0	54090390	3123	Reach_4920	2775	269	100.0	4.8E-03	1.2E-01	9.1E+04									18%	-9.2	-9.5	-11.2
tert-butyl 3-[6-({[1-(2,2-difluoro-1,3-benzodioxol-5-yl)cyclopro	204-501-7	121-86-8	121868	376	Reach_1020	2776	172	56.5	8.6E-01	7.6E+01	1.0E+03	0	0	3.3E-09	3.5E-08	1.1E-07				15%	-8.6	-9.5	-11.3
phthalylsulfathiazole	696-555-7	32454-35-6	32454356	2652	Reach_4719	2777	243	103.2	1.5E-02	1.1E+02	1.5E+03	4.18	0	1.1E-06	1.1E-07	3.5E-07				14%	-8.8	-9.5	-11.4
620-459-6	620-459-6	130841-23-5	130841235	1844	Reach_4569	2778	358	95.1	6.3E-02	2.5E-01	3.0E+05			1.1E-06	1.1E-07	3.5E-07				19%	-9.8	-9.5	-11.4
N-[2-[(2-hydroxyethyl)amino]ethyl]dodecanamide	235-930-8	13051-49-5	13051495	1838	Reach_2321	2779	179	8.7	1.7E+01	2.1E+03	3.0E+00	0	0	3.5E-06	3.5E-07	1.1E-06				15%	-8.8	-9.5	-11.4
4-(4-iodo-1H-pyrazol-1-yl)piperidine	609-304-3	368890-20-4	368890204	2784	Reach_4296	2780	372	226.3	4.5E-09	6.0E-01	1.1E+04		10.1	1.1E-06	1.1E-07	3.5E-07				14%	-8.8	-9.5	-11.4
N-phenylbenzenesulphonamide	608-993-8	34455-22-6	34455226	2707	Reach_4286	2781	512	105.7	2.5E-02	6.6E+00	4.2E+04	8.65		1.1E-06	3.5E-08	3.5E-07				15%	-9.0	-9.5	-11.4
1-[(2E)-3,7-dimethylocta-2,6-dien-1-yl]pyrrolidine-2,5-dione	800-131-0	104372-31-8	104372318	1392	Reach_5037	2782	229	121.2	1.4E-02	6.5E+03	4.5E+02		0	3.5E-07	3.5E-08	1.1E-07				15%	-8.8	-9.5	-11.4
(E)-3,7-dimethylocta-2,6-dienal	219-194-5	2385-77-5	2385775	2361	Reach_1791	2783	154	-28.3	3.4E+01	2.9E+02	3.4E+03			1.1E-06	3.5E-07	1.1E-06				15%	-9.8	-9.5	-11.2
(Z)-3,7-dimethylocta-2,6-dienal	205-476-5	141-27-5	141275	1935	Reach_1160	2784	152	-26.7	1.2E+01	8.6E+02	2.8E+03			3.5E-06	1.1E-06	3.5E-06				15%	-9.8	-9.5	-11.2
tetradecyl acrylate	244-491-1	21643-42-5	21643425	2302	Reach_2507	2785	268	62.0	3.3E-02	7.6E-02	1.3E+07			1.1E-06	1.1E-07	3.5E-07				21%	-9.6	-9.5	-11.3
cyclohexanethiol	216-378-7	1569-69-3	1569693	2054	Reach_1695	2786	116	-45.3	3.5E+02	6.6E+02	1.1E+03	10.7		3.5E-07	1.1E-07	3.5E-07				18%	-9.8	-9.5	-11.3
bromoethane	600-588-4	104617-50-7	104617507	5593	Reach_4069	2787	292	0.0												24%	-9.8	-9.5	-12.0
1-methylnaphthalene	201-966-8	90-12-0	90120	1000	Reach_359	2788	142	22.2	4.9E+00	4.0E+01	5.2E+03			3.3E-08	3.5E-08	1.1E-07				22%	-9.8	-9.5	-10.9
2,6,10-Trimethyldodecane	622-542-2	3891-98-3	3891983	2829	Reach_4576	2789	212	-19.8	1.7E+01	1.0E-03	3.1E+07			3.5E-07	3.5E-08	1.1E-07				23%	-9.7	-9.5	-11.9
butane-2,3-diol	208-173-6	513-85-9	513859	3038	Reach_1318	2790	90	-34.4	2.3E+01	1.5E+06	4.4E-01	14.9		3.5E-06	1.1E-06	3.5E-06				14%	-9.2	-9.5	-11.5
furan	202-458-9	95-85-2	95852	4136	Reach_445	2791	144	69.8	3.4E-02	7.4E+03	1.7E+01			1.1E-06	1.1E-07	3.5E-07				24%	-9.9	-9.5	-11.9
hexachloroacetone	217-285-4	1798-60-3	1798603	2162	Reach_1721	2792	150	39.5	1.6E-01	3.7E+04	7.1E+00			3.5E-06	3.5E-07	1.1E-06				23%	-9.9	-9.5	-11.8
2,4-dichloro-α,α,α-trifluorotoluene	610-122-1	433733-94-9	433733949	2910	Reach_4321	2793	326	226.1	4.7E-09	2.7E+02	7.9E-01			3.5E-06	3.5E-07	1.1E-06				23%	-9.8	-9.5	-12.1
4-methyl-N-[3-(4-methyl-1H-imidazol-1-yl)-5-(trifluoromethyl)p	613-879-6	66069-32-7	66069327	5977	Reach_4388	2794	328	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				16%	-8.8	-9.5	-11.3
615-790-8	615-790-8	72714-62-6	72714626	3610	Reach_4417	2795	330	43.2	2.7E+00	1.6E+00	2.5E+05			3.5E-06	3.5E-07	1.1E-06				19%	-9.8	-9.5	-12.2
heptan-2-one	203-767-1	110-43-0	110430	278	Reach_814	2796	114	-42.8	6.5E+02	2.4E+03	5.4E+01			9.4E-07	1.1E-07	3.5E-07				15%	-9.8	-9.5	-11.2
2,3,4,5-tetrafluorobenzoyl chloride	610-950-3	53056-20-5	53056205	3085	Reach_4340	2797	223	64.3	4.0E-01	1.4E+01	3.3E+02			1.1E-07	1.1E-08	3.5E-08				16%	-9.8	-9.5	-11.7
dibutyl sebacate	203-672-5	109-43-3	109433	1500	Reach_773	2798	314	-6.8	2.4E-02	7.8E-01	2.0E+06			1.1E-06	1.1E-07	3.5E-07				20%	-9.7	-9.5	-11.0
3,3-dimethylbutyryl chloride	201-901-3	89-36-1	89361	3972	Reach_341	2799	254	196.6	4.3E-09	3.7E+03	2.5E-01			1.1E-06	1.1E-07	3.5E-07				16%	-9.8	-9.5	-11.5
600-558-0	220-836-1	2915-57-3	2915573	2559	Reach_1884	2800	343	-12.1	1.3E-02	2.9E-01	1.3E+07			1.1E-06	1.1E-07	3.5E-07				20%	-9.7	-9.5	-11.2
3-fluorotoluene	277-730-3	74124-79-1	74124791	3632	Reach_2942	2801	256	240.3	5.3E-10	1.0E+06	1.7E-05			1.1E-06	3.5E-07	1.1E-06				21%	-9.8	-9.5	-11.9
3-(diethoxymethylsilyl)propylamine	217-284-9	1798-50-1	1798501	5746	Reach_1720	2802	304	0.0	0.0E+00	0.0E+00	0.0E+00		0	0.0E+00	0.0E+00	0.0E+00				14%	-9.8	-9.5	-11.4
dimethylsulphamoyl chloride	801-489-0	128346-46-3	128346463	5653	Reach_5056	2803	230	0.0												14%	-9.8	-9.5	-11.4
methyl 3-α,7-α-diacetoxy-12-α-hydroxy-5-β-cholan-24-oate	223-151-6	3749-87-9	3749879	2800	Reach_1989	2804	507	201.8	1.3E-10	5.7E-01	2.6E+05	15.8		1.1E-06	1.1E-07	3.5E-07				18%	-8.8	-9.5	-11.2
1,3-diphenylpropane-1,3-dione	204-398-9	120-46-7	120467	1712	Reach_994	2805	224	106.9	6.3E-03	1.3E+02	3.2E+02	8.3		1.1E-06	1.1E-07	3.5E-07				15%	-9.7	-9.5	-11.4
1,2,3-trichloro-5-(trifluoromethyl)benzene	608-991-7	344348-40-9	344348409	2705	Reach_4285	2806	216	67.0	5.4E-02	1.5E+01	1.4E+04			3.5E-07	1.1E-07	3.5E-07				23%	-9.8	-9.5	-12.2
m-tolyl isocyanate	252-021-1	34432-92-3	34432923	2704	Reach_2677	2807	370	159.5	5.4E-06	1.9E-02	1.1E+06			3.5E-06	1.1E-07	3.5E-07				15%	-9.8	-9.5	-11.0
617-345-3	282-716-5	84332-87-6	84332876	6050	Reach_2971	2808	260	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				16%	-8.8	-9.5	-11.3
617-351-6	617-712-8	85448-44-8	85448448	6059	Reach_4473	2809	556	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				16%	-8.8	-9.5	-11.3
toluene-2-sulphonamide	201-808-8	88-19-7	88197	3951	Reach_319	2810	171	91.2	8.1E-03	2.3E+03	8.3E+00	10.1		3.5E-07	3.5E-08	1.1E-07				16%	-8.9	-9.5	-11.4
bis(3,5,5-trimethylhexanoyl) peroxide	223-356-0	3851-87-4	3851874	2823	Reach_1995	2811	314	6.8	2.0E-01	1.8E-01	1.1E+07			1.1E-06	3.5E-07	1.1E-06				22%	-9.6	-9.5	-11.7
1,4,7-triazonanetriium sulfate (2:3)	700-907-8	220493-36-7	220493367	5778	Reach_5023	2812	553	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.2	-9.5	-11.2
604-106-3	202-709-2	98-87-3	98873	4195	Reach_522	2813	161	-13.9	3.7E+01	9.9E+01	9.3E+02		0	3.5E-07	3.5E-08	1.1E-07				15%	-9.8	-9.5	-11.4
617-344-8	278-757-3	77743-24-9	77743249	6035	Reach_2950	2814	663	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				16%	-8.8	-9.5	-11.3
2-chloro-6-fluorotoluene	688-269-6	641571-11-1	641571111	3428	Reach_4642	2815	241	136.7	3.9E-04	2.6E+02	2.6E+02			1.1E-06	1.1E-07	3.5E-07				21%	-9.9	-9.5	-12.0
methyl (S)-(-)-lactate	251-846-4	34140-91-5	34140915	5850	Reach_2671	2816	890	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-9.7	-9.5	-11.5
614-477-3	245-910-0	23847-08-7	23847087	2360	Reach_2536	2817	288	198.8	3.0E-07	4.9E+02	9.5E+00			3.5E-07	3.5E-08	1.1E-07				18%	-9.7	-9.5	-11.2
canrenone	603-835-4	134568-16-4	134568164	1879	Reach_4130	2818	184	67.0	3.7E-01	3.4E+03	1.1E+01			3.5E-06	1.1E-07	3.5E-07				17%	-8.9	-9.5	-11.3
4-bromoanisole	203-252-1	104-92-7	104927	1402	Reach_633	2819	187	11.1	2.3E+01	3.2E+02	9.1E+02			3.5E-07	1.1E-07	3.5E-07				17%	-9.8	-9.5	-11.0
tetrahydrofuran-3-carbaldehyde	209-193-8	558-30-5	558305	3180	Reach_1372	2820	72	-79.0	3.8E+04	6.3E+04	6.8E+00			1.1E-06	1.1E-07	3.5E-07				14%	-9.8	-9.5	-11.2
methyl laurate	203-911-3	111-82-0	111820	1559	Reach_873	2821	214	23.2	1.5E+00	1.5E+00	1.9E+05			1.1E-06	1.1E-07	3.5E-07				19%	-9.8	-9.5	-11.7
610-979-1	617-351-6	82544-13-6	82544136	3832	Reach_4458	2822	417	199.8	2.4E-09	3.4E+00	9.1E+03			1.1E-06	1.1E-07	3.5E-07				16%	-9.8	-9.5	-11.0
1,4-bis[chloro(difluoro)methyl]benzene	800-301-4	862574-88-7	862574887	3901	Reach_5042	2823	242	125.4	3.3E-03	7.5E+02	6.6E+03			1.1E-06	1.1E-07	1.1E-06				22%	-9.8	-9.5	-12.1
2-methylnaphthalene	203-224-9	104-66-5	104665	1397	Reach_625	2824	214	71.1	2.2E-02	2.8E+01	6.5E+03			3.5E-07	1.1E-07	3.5E-07				22%	-9.8	-9.5	-11.2
1-bromopentane	211-684-7	685-88-1	685881	3520	Reach_1501	2825	178	-93.7	4.2E+02	5.4E+03	5.8E+00			3.5E-06	3.5E-07	1.1E-06				22%	-9.9	-9.5	-12.1
disodium 6-acetamido-4-hydroxy-3-[[4-[[2-(sulphonatooxy)eth	243-653-9	20262-58-2	20262582	5766	Reach_2490	2826	618	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.2	-9.5	-11.2
N-(1-oxooctyl)glycine	238-122-3	14246-53-8	14246538	1956	Reach_2361	2827	201	149.9	1.3E-04	1.8E+02	8.3E+01	3.5		1.1E-06	3.5E-07	1.1E-06				14%	-8.9	-9.6	-11.5

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
2,5,7,10-tetraoxaundecane	213-554-5	976-71-6	976716	4170	Reach_1623	2828	340	188.4	2.5E-06	4.1E+01	1.1E+04			3.5E-07	3.5E-08	1.1E-07				16%	-9.8	-9.6	-11.3
cycloocta-1,5-diene	613-975-8	666816-98-4	666816984	3477	Reach_4392	2829	297	239.4	6.0E-10	7.9E+00	3.9E+01			3.5E-07	3.5E-08	1.1E-07				24%	-9.9	-9.6	-11.9
dichloroacetyl chloride	201-199-9	79-36-7	79367	3772	Reach_241	2830	147	-32.5	3.5E+03	1.2E+03	9.1E-01			1.1E-07	1.1E-08	3.5E-08				22%	-10.0	-9.6	-12.0
4-(methylthio)-m-cresol	209-842-5	594-44-5	594445	3277	Reach_1399	2831	129	4.4	1.7E+02	3.1E+04	5.8E+01			3.5E-06	3.5E-07	1.1E-06				14%	-9.8	-9.6	-11.4
androsta-1,4-diene-3,17-dione	212-977-2	897-06-3	897063	3983	Reach_1587	2832	284	146.1	3.0E-04	1.9E+01	3.5E+02			3.5E-07	1.1E-07	3.5E-07				16%	-9.6	-9.6	-11.4
4-amino-N-[4-(aminocarbonyl)phenyl]benzamide	277-874-7	74441-06-8	74441068	3636	Reach_2944	2833	255	227.8	3.6E-09	1.5E+01	3.4E+00	14.5	11.6	1.1E-06	3.5E-07	1.1E-06				14%	-8.5	-9.6	-11.5
1-bromodecane	222-423-1	3467-59-2	3467592	2712	Reach_1966	2834	195	129.2	1.3E-03	4.4E+03	5.0E+00			1.1E-06	1.1E-07	3.5E-07				22%	-9.8	-9.6	-12.4
2-nitrobenzaldehyde	209-025-3	552-89-6	552896	697	Reach_1360	2835	151	69.5	8.4E-01	1.1E+03	3.4E+01			8.7E-07	3.5E-08	1.1E-07				15%	-9.8	-9.6	-11.5
α,α,α,β,β,β-hexafluoro-m-xylene	207-300-2	460-00-4	460004	2946	Reach_1282	2836	175	-19.1	5.0E+02	2.3E+02	1.2E+03			3.5E-07	3.5E-08	1.1E-07				22%	-9.9	-9.6	-12.3
norethisterone	603-746-0	13349-82-1	13349821	1867	Reach_4127	2837	174	89.5	5.2E-03	1.0E+06	1.4E-02	14.9		1.1E-06	3.5E-07	1.1E-06				17%	-8.9	-9.6	-11.3
benzylidene(methyl)amine	210-728-2	622-29-7	622297	3364	Reach_1444	2838	119	-39.1	1.0E+02	1.4E+03	5.0E+01		7.9	3.5E-07	3.5E-08	1.1E-07				16%	-9.8	-9.6	-10.9
dichloro(methyl)(vinyl)silane	204-710-3	124-70-9	124709	1793	Reach_1082	2839	141	-78.5	6.9E+03		4.0E+02			1.1E-06	1.1E-07	3.5E-07				19%	-9.9	-9.6	-12.3
2-methoxyethyl acrylate	221-499-3	3121-61-7	3121617	2621	Reach_1919	2840	130	-40.2	6.0E+02	4.5E+04	2.8E+00			3.5E-06	3.5E-07	1.1E-06				14%	-9.8	-9.6	-11.3
613-941-2	260-252-4	56539-66-3	56539663	3201	Reach_2816	2841	118	-25.3	1.0E+02	1.5E+05	2.9E+00			1.1E-06	3.5E-07	1.1E-06				14%	-9.8	-9.6	-11.3
benzil	205-157-0	134-81-6	134816	1883	Reach_1128	2842	210	98.6	4.4E-03	6.0E+00	3.6E+03			1.1E-06	1.1E-07	3.5E-07				15%	-9.8	-9.6	-11.4
4,10-dibromodibenzo[def,mno]chrysene-6,12-dione	204-984-4	130-26-7	130267	1834	Reach_1118	2843	306	134.4	4.8E-05	3.0E+01	3.0E+03			1.1E-06	1.1E-07	3.5E-07				22%	-9.4	-9.6	-10.8
dodecyl methyl sulphide	241-972-8	18063-03-1	18063031	2163	Reach_2450	2844	157	84.7	3.8E-02	1.3E+03	1.0E+00			1.1E-06	3.5E-07	1.1E-06				23%	-9.8	-9.6	-12.3
propionyl chloride	201-170-0	79-03-8	79038	3764	Reach_224	2845	93	-67.5	1.3E+04	1.9E+04	1.0E+00			3.5E-06	1.1E-06	3.5E-06				14%	-9.9	-9.6	-11.7
trans-1-(1-oxohexadecyl)-4-[(1-oxohexadecyl)oxy]-L-proline	255-490-0	41672-81-5	41672815	2882	Reach_2746	2846	608	298.6	5.3E-14	2.9E-08	1.6E+13	2.99		1.1E-06	1.1E-07	3.5E-07				21%	-9.8	-9.6	-10.2
octahydrocyclopenta[c]pyrrole	227-114-5	5661-03-0	5661030	3206	Reach_2131	2847	111	6.8	2.3E+02	1.5E+05	3.7E+01		3.1	1.1E-06	3.5E-08	1.1E-07				14%	-9.8	-9.6	-11.4
sodium (4,6-dimethoxypyrimidin-2-yl)({[3-(2,2,2-trifluoroethox	700-684-7	80793-17-5	80793175	3798	Reach_4967	2848	348	-67.1	9.9E+03	2.3E-02	7.4E+05									18%	-9.3	-9.6	-11.2
612-101-2	608-356-4	2941-20-0	2941200	2564	Reach_4272	2849	135	11.3	2.7E+01	1.5E+03	9.5E+01			3.5E-07	3.5E-08	1.1E-07				23%	-9.8	-9.6	-12.1
N-amidinosarcosine	203-581-0	108-42-9	108429	238	Reach_744	2850	128	24.4	1.0E+01	1.7E+03	5.2E+01	0	10	6.5E-09	1.1E-07	3.5E-07				14%	-8.4	-9.6	-11.7
phenolphthalein	201-004-7	77-09-8	77098	879	Reach_179	2851	318	218.4	8.4E-11	3.2E+01	1.1E+03	9.43		1.1E-07	1.1E-07	3.5E-07				19%	-9.1	-9.6	-11.1
2-(trifluoromethyl)benzenesulfonyl chloride	205-319-0	138-24-9	138249	5684	Reach_1140	2852	172	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				17%	-9.8	-9.6	-11.1
N-[3-(trimethoxysilyl)propyl]butylamine	242-272-5	18395-30-7	18395307	2188	Reach_2461	2853	178	-34.5	4.5E+02	2.7E+03	5.4E+00		0	1.1E-06	3.5E-07	1.1E-06				14%	-9.8	-9.6	-11.7
620-225-3	617-339-0	824-80-6	824806	6044	Reach_4450	2854	182	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				19%	-9.1	-9.6	-11.1
604-112-6	211-910-4	709-55-7	709557	3576	Reach_1519	2855	181	96.5	2.8E-04	4.3E+04	1.9E+00			1.1E-05	1.1E-06	3.5E-06				23%	-9.9	-9.6	-12.3
bromomethane	200-813-2	74-83-9	74839	837	Reach_109	2856	95	-105.4	2.1E+05	1.2E+04	1.5E+01			4.3E-08	3.5E-08	1.1E-07				23%	-10.0	-9.6	-12.1
2-(2-butoxyethoxy)ethyl methacrylate	230-813-8	7328-22-5	7328225	3618	Reach_2238	2857	230	35.5	7.1E-01	1.3E+03	1.6E+02			1.1E-06	3.5E-07	1.1E-06				15%	-9.9	-9.6	-11.5
605-830-2	204-203-7	117-69-1	117691	1663	Reach_960	2858	534	349.8	3.4E-25	9.1E-06	5.0E+01			3.5E-07	3.5E-08	1.1E-07				14%	-8.5	-9.6	-11.8
ethyl 2-chloropropionate	202-266-5	93-67-4	93674	4077	Reach_404	2859	220	113.1	3.3E-03	8.6E+00	8.7E+02			3.5E-07	3.5E-08	1.1E-07				14%	-9.9	-9.6	-11.3
617-546-6	617-546-6	84170-74-1	84170741	3857	Reach_4466	2860	328	19.9	2.2E-02	2.8E+01	8.1E+02			3.5E-06	3.5E-07	1.1E-06				14%	-9.9	-9.6	-11.5
tetrahydrocyclopenta[c]pyrrole-1,3(2H,3aH)-dione	606-984-3	22327-32-8	22327328	2330	Reach_4231	2861	150	28.9	2.9E+01	2.9E+03	7.1E+02	0		1.1E-06	3.5E-07	1.1E-06				14%	-8.5	-9.6	-11.8
tert-butyl (6S)-6-[4-(7-bromo-9,9-difluoro-9H-fluoren-2-yl)-1H-	204-005-0	112-77-6	112776	1603	Reach_924	2862	301	93.9	6.1E-03	2.8E-03	1.5E+07	0	0	1.1E-06	1.1E-07	3.5E-07				18%	-9.1	-9.6	-11.3
dibutylbis(dodecylthio)stannane	214-688-7	1185-81-5	1185815	6392	Reach_1667	2863	636	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.3	-9.6	-11.3
α,α-bis[4-(dimethylamino)phenyl]-4-(phenylamino)naphthalen	229-851-8	6786-83-0	6786830	3502	Reach_2206	2864	488	275.6	2.7E-15	5.7E-04	1.6E+07		8.09	3.5E-07	1.1E-08	3.5E-08				21%	-9.2	-9.6	-11.1
diethyl phenylphosphonite	700-781-4	160332-89-8	160332898	5729	Reach_4993	2865	543	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				16%	-9.9	-9.6	-11.0
naphthalene-1,5-diol	239-350-6	15308-01-7	15308017	2030	Reach_2384	2866	315	155.6	1.9E-05	7.4E-01	5.5E+03	0		1.1E-07	1.1E-08	3.5E-08				14%	-8.7	-9.6	-11.6
acenaphthene	201-469-6	83-32-9	83329	952	Reach_281	2867	154	53.6	1.7E-01	5.2E+00	1.4E+04			1.2E-08	3.5E-08	1.1E-07				23%	-9.9	-9.6	-10.8
605-954-7	209-282-1	565-61-7	565617	3203	Reach_1376	2868	100	-66.7	2.7E+03	9.6E+03	1.4E+01			1.1E-06	3.5E-07	1.1E-06				15%	-9.9	-9.6	-11.4
[4-(2-hydroxyethoxy)-1,3-phenylene]diammonium sulphate	274-713-2	70643-20-8	70643208	6005	Reach_2919	2869	266	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.3	-9.6	-11.3
617-708-6	214-371-3	1123-25-7	1123257	1582	Reach_1661	2870	142	51.9	6.4E+00	1.9E+03	6.5E+02	4.9		3.5E-06	3.5E-07	1.1E-06				17%	-8.8	-9.6	-11.3
2-thienylacetonitrile	227-998-2	6065-63-0	6065630	3314	Reach_2152	2871	244	-20.3	1.9E+00	2.7E+02	5.4E+03			3.5E-06	3.5E-07	1.1E-06				14%	-9.8	-9.6	-11.3
dimethyl(propyl)amine	213-139-9	926-63-6	926636	4042	Reach_1598	2872	87	-83.4	2.1E+04	1.4E+05	1.0E+01		3.9	3.5E-06	3.5E-07	1.1E-06				14%	-9.9	-9.6	-11.3
619-817-4	619-817-4	52671-72-4	52671724	3067	Reach_4548	2873	286	215.9	2.2E-08	4.9E+01	1.0E+03	2.13		1.1E-06	1.1E-07	3.5E-07				14%	-9.0	-9.6	-11.6
dodecanal	203-983-6	112-54-9	112549	333	Reach_912	2874	184	13.8	2.1E+00	4.0E+00	5.6E+04			3.7E-06	3.5E-08	1.1E-07				17%	-9.9	-9.6	-11.7
1,3,3-trimethyl-N-(2-methylpropylidene)-5-[(2-methylpropylide	200-832-6	75-02-5	75025	3655	Reach_124	2875	46	-148.2	1.7E+06	2.8E+04	1.5E+01		0	1.1E-06	1.1E-07	3.5E-07				22%	-9.7	-9.6	-10.6
606-356-9	617-931-9	868-84-8	868848	3912	Reach_4480	2876	122	-20.0	1.3E+02	4.4E+03	1.0E+01			3.5E-07	3.5E-08	3.5E-07				15%	-9.9	-9.6	-11.1
3-methylpent-3-en-2-one	209-283-7	565-62-8	565628	3204	Reach_1377	2877	98	-64.4	2.5E+03	1.3E+04	2.3E+01			1.1E-06	3.5E-07	1.1E-06				15%	-9.9	-9.6	-11.2
4,5-dimethyl-2-(propan-2-yl)phenol	255-982-5	42872-30-0	42872300	2902	Reach_2753	2878	235	125.9	3.5E-04	9.0E+00	1.3E+03	0		1.1E-06	1.1E-07	3.5E-07				16%	-9.8	-9.6	-11.4
(Z)-3-hexenyl salicylate	265-745-8	65405-77-8	65405778	3452	Reach_2872	2879	220	99.5	2.6E-03	2.0E+00	6.9E+04	9.8		1.1E-06	1.1E-07	3.5E-07				17%	-9.8	-9.6	-11.4
4,6-Dichloro-2-ethoxypyrimidine	282-810-6	84434-11-7	84434117	3864	Reach_2974	2880	316	84.9	7.1E-05	2.5E+00	1.3E+03			1.1E-06	3.5E-08	1.1E-07				15%	-9.9	-9.6	-11.3
buta-1,2-diene	209-865-0	595-37-9	595379	738	Reach_1400	2881	116	21.6	9.6E+01	3.1E+04	8.7E+01			2.2E-09	3.5E-07	1.1E-06				20%	-9.9	-9.6	-12.4
(1S)-1-(2,6-dichloro-3-fluorophenyl)ethanol	619-997-4	764667-65-4	764667654	3712	Reach_4555	2882	406	181.1	4.2E-06	3.6E+01	1.2E+02	8.27		3.5E-07	3.5E-08	1.1E-07				19%	-9.9	-9.6	-11.1
p-tolyl isocyanate	242-616-4	18835-34-2	18835342	2211	Reach_2470	2883	393	132.9	5.3E-05	6.8E-10	9.1E+13			1.1E-06	1.1E-07	3.5E-07				15%	-9.9	-9.6	-11.0
800-940-9	800-940-9	35836-72-7	35836727	2750	Reach_5049	2884	208	54.2	1.2E+00	1.4E+03	2.0E+04			3.5E-06	3.5E-07	1.1E-06				16%	-9.8	-9.6	-11.5
ethyl difluoroacetate	619-799-8	66309-83-9	66309839	3468	Reach_4546	2885	160	59.5	7.9E-01	2.5E+02	1.2E+03			3.5E-07	3.5E-08	1.1E-07				14%	-9.9	-9.6	-11.5
4-tert-butylcyclohexyl chloroformate	207-787-1	494-19-9	494199	2980	Reach_1295	2886	195	103.5	9.3E-03	5.5E-02	1.9E+04			3.5E-07	3.5E-08	1.1E-07				20%	-9.9	-9.6	-12.3
isopropyl 2-bromo-2-methylpropionate	257-158-0	51368-55-9	51368559	3037	Reach_2772	2887	209	-10.8	1.1E+02	2.6E+02	3.2E+02			3.5E-06	3.5E-07	1.1E-06				15%	-9.9	-9.6	-11.8
(R)-3,7-dimethyloct-6-enal	203-379-2	106-26-3	106263	1433	Reach_663	2888	152	-26.7	1.2E+01	8.6E+02	2.8E+03			3.5E-06	1.1E-06	3.5E-06				16%	-9.9	-9.6	-11.1
butan-2-one O,O',O'',O'''-silanetetrayltetraoxime	251-882-0	34206-40-1	34206401	2694	Reach_2673	2889	373	42.1	1.3E-03	7.9E-01	1.2E+12			3.5E-07	1.1E-07	3.5E-07				24%	-9.8	-9.6	-10.1
5-sulphoisophthalic acid	221-696-4	3195-24-2	3195242	2640	Reach_1931	2890	240	-22.8	5.1E+00	9.2E+01	2.9E+03	0		3.5E-06	3.5E-07	1.1E-06				14%	-8.5	-9.6	-11.8
propane-1,2,3-triyl 2-ethylhexanoate	230-896-0	7360-38-5	7360385	3624	Reach_2241	2891	471	73.0	2.4E-05	1.1E-02	9.5E+08			1.1E-06	1.1E-07	3.5E-07				23%	-9.4	-9.6	-10.3
1-[4-(Chlorocarbonyl)benzyl]-4- methylpiperazinediium dichlor	220-165-4	2649-76-5	2649765	2472	Reach_1851	2892	371	187.0	8.7E-07	4.5E-01	7.8E+04									18%	-9.3	-9.6	-11.3
nadide	200-184-4	53-84-9	53849	3113	Reach_21	2893	663	90.3	2.7E-09	2.9E+03	6.3E-07	0.28	10.4	3.5E-07	1.1E-07	3.5E-07				16%	-8.6	-9.6	-11.6
3,4-dichloro-N-(5-chloro-2-hydroxy-4-nitrophenyl)benzamide	601-327-7	114772-54-2	114772542	1625	Reach_4083	2894	272	131.5	2.8E-04	3.3E-01	1.5E+04	0		3.5E-07	3.5E-08	3.5E-08				18%	-9.0	-9.6	-11.3
isopropenyl methyl ether	604-075-6	138401-24-8	138401248	4396	Reach_4140	2895	386	243.5	3.2E-10	5.6E-03	4.6E+06			1.1E-06	3.5E-08	1.1E-07				17%	-9.9	-9.6	-12.0
1,3-diisopropylbenzene	202-773-1	99-62-7	99627	4210	Reach_534	2896	162	-16.1	4.1E+01	1.2E+00	7.9E+04			3.5E-07	3.5E-08	1.1E-07				23%	-9.9	-9.6	-12.3
3,3,10,10-tetramethoxy-2,11-dioxa-3,10-disiladodecane	617-969-6	87135-01-1	87135011	3918	Reach_4482	2897	327	73.7	6.9E-02	1.1E+02	1.9E+00			3.5E-07	1.1E-07	3.5E-07				16%	-9.9	-9.6	-11.4
dodecyl acrylate	218-463-4	2156-97-0	2156970	533	Reach_1765	2898	240	34.4	2.7E-01	4.3E-02	1.3E+06			5.6E-07	1.1E-07	3.5E-07				22%	-9.9	-9.6	-12.1
sodium 8-phenylamino-5-(4-(3-sulphonatophenylazo)-1-naphtl	600-553-3	10429-07-9	10429079	1389	Reach_4067	2899	445	229.6	2.7E-09	6.2E+02	1.4E+05									18%	-9.3	-9.6	-11.3
4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol	209-218-2	561-41-1	561411	3187	Reach_1373	2900	376	208.6	5.2E-10	4.9E-01	2.3E+04		7.74	1.1E-06	3.5E-07	1.1E-06				15%	-8.9	-9.6	-11.4
N-(4-amino-5-chloro-2-hydroxyphenyl)-3,4-dichlorobenzamide	600-198-4	101377-47-3	101377473	1319	Reach_4057	2901	315	143.6	3.0E-04	0.0E+00	7.8E+04	0	12.1	1.1E-06	1.1E-07	3.5E-07				14%	-9.0	-9.6	-11.8
betamethasone	206-825-4	378-44-9	378449	619	Reach_1261	2902	392	216.8	7.7E-12	6.5E+01	5.2E+01	13		1.0E-07	3.5E-07	1.1E-06				19%	-9.1	-9.6	-11.1

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
trichloroisobutylsilane	242-053-4	18169-57-8	18169578	2171	Reach_2454	2903	192	-50.6	7.3E+02	4.8E+03	2.6E+03			3.5E-06	1.1E-06	3.5E-06				15%	-9.9	-9.6	-11.6
isopentyl p-methoxycinnamate	275-702-5	71617-10-2	71617102	3587	Reach_2929	2904	248	72.4	2.5E-02	5.9E+00	2.1E+04			1.1E-06	1.1E-07	3.5E-07				16%	-9.9	-9.6	-11.3
tert-pentyl hydroperoxide	222-321-7	3425-61-4	3425614	2698	Reach_1959	2905	104	-28.9	1.8E+03	1.0E+05	2.7E+01	12.7		1.1E-06	3.5E-07	1.1E-06				14%	-9.9	-9.6	-11.1
di-tert-butyl 3,3,5-trimethylcyclohexylidene diperoxide	229-782-3	6731-36-8	6731368	3488	Reach_2205	2906	302	86.3	2.5E+04	4.6E-01	3.6E+07			3.5E-07	3.5E-08	1.1E-07				23%	-9.8	-9.6	-11.9
octamethyltrisiloxane	203-497-4	107-51-7	107517	1464	Reach_710	2907	237	-53.2	4.7E+02	6.2E-01	5.0E+06			3.5E-09	3.5E-09	3.5E-09				24%	-10.0	-9.6	-12.2
2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclotetrasiloxane	219-863-1	2554-06-5	2554065	1252	Reach_1839	2908	345	42.4	1.4E+01	0.0E+00	1.6E+08			1.1E-06	1.1E-07	3.5E-07				23%	-9.5	-9.6	-11.7
trimethoxy(2,4,4-trimethylpentyl)silane	251-995-5	34396-03-7	34396037	2702	Reach_2676	2909	234	7.3	2.2E+01	1.1E+02	3.8E+02			3.5E-07	1.1E-07	3.5E-07				18%	-9.9	-9.6	-11.4
estradiol	200-023-8	50-28-2	50282	55	Reach_7	2910	272	152.4	2.7E-07	8.8E+00	8.7E+03	10		9.5E-08	3.5E-07	1.1E-06				20%	-9.1	-9.6	-11.1
4-amino-2,5-dichloro-N,N-dimethylbenzenesulphonamide	606-682-1	2098-65-9	2098659	2281	Reach_4212	2911	791	349.8	1.8E-24	7.5E-06	3.5E+07		11.8	1.1E-06	1.1E-07	3.5E-07				16%	-8.7	-9.6	-11.5
1-[(2,4-dinitrophenyl)azo]-2-naphthol	222-429-4	3468-63-1	3468631	2713	Reach_1967	2912	338	220.9	1.2E-09	1.9E-01	5.2E+05	8.5		3.5E-06	3.5E-08	1.1E-07				18%	-9.1	-9.7	-11.4
disodium 7-benzamido-4-hydroxy-3-[[4-[(4-sulphonatophenyl)	220-028-9	2610-11-9	2610119	1182	Reach_1845	2913	676	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.3	-9.7	-11.3
617-834-1	696-107-0	930086-71-8	930086718	6084	Reach_4705	2914	420	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				17%	-9.4	-9.7	-11.4
dimethyl 2-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amin	252-650-1	35636-63-6	35636636	2742	Reach_2692	2915	453	287.8	3.0E-13	3.8E+01	7.6E+01	8.57	12	1.1E-06	1.1E-07	3.5E-07				14%	-8.8	-9.7	-11.7
tert-butyl 3,5,5-trimethylperoxyhexanoate	236-050-7	13122-18-4	13122184	1847	Reach_2323	2916	230	21.3	7.0E+00	2.6E+00	4.9E+04			3.5E-06	3.5E-07	1.1E-06				18%	-9.9	-9.7	-12.4
trimethyl phosphonoacetate	227-663-0	5927-18-4	5927184	3272	Reach_2145	2917	182	9.1	7.1E+00	1.0E+05	5.8E-01			3.5E-06	3.5E-07	1.1E-06				14%	-9.8	-9.7	-11.7
cyclohexene	203-807-8	110-83-8	110838	286	Reach_831	2918	82	-81.4	1.1E+04	2.6E+02	9.1E+02			8.2E-08	1.1E-07	3.5E-07				23%	-10.0	-9.7	-12.3
N,N-dimethylisopropylamine	213-635-5	996-35-0	996350	4211	Reach_1629	2919	87	-95.4	2.1E+04	1.4E+05	8.9E+00		3.8	3.5E-06	3.5E-07	1.1E-06				14%	-9.9	-9.7	-11.4
3,3'-dimethylbiphenyl-4,4'-diyl diisocyanate	202-112-7	91-97-4	91974	4025	Reach_382	2920	264	116.0	2.9E-03	7.1E+00	1.1E+06			1.1E-06	3.5E-08	1.1E-07				20%	-9.7	-9.7	-11.3
3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctan-1-ol	211-477-1	647-42-7	647427	3443	Reach_1485	2921	364	-16.4	1.3E+02	2.1E-01	2.6E+04	13.5		3.5E-06	1.1E-06	3.5E-06				19%	-9.9	-9.7	-12.9
methyl (R)-lactate	241-420-6	17392-83-5	17392835	2134	Reach_2432	2922	104	-39.8	2.4E+02	3.4E+05	2.1E-01	12.6		3.5E-06	3.5E-07	1.1E-06				14%	-9.9	-9.7	-11.6
methyl bromoacetate	202-499-2	96-32-2	96322	4144	Reach_461	2923	153	-42.2	1.2E+03	3.8E+05	5.2E+00			3.5E-06	3.5E-07	1.1E-06				14%	-9.9	-9.7	-11.5
N,N'-(3,3'-dimethylbiphenyl-4,4'-ylene)di(acetoacetamide)	202-111-1	91-96-3	91963	4024	Reach_381	2924	380	277.3	1.5E-04	2.5E+01	5.6E+01	10.4	13.1	1.1E-06	1.1E-07	3.5E-07				14%	-8.9	-9.7	-11.7
2-aminophenol	202-431-1	95-55-6	95556	4127	Reach_434	2925	109	53.6	6.7E-02	5.6E+04	4.0E+00	10.3	9.4	3.5E-06	1.1E-07	1.1E-06				14%	-8.7	-9.7	-11.7
trisodium 1-(1-naphthylazo)-2-hydroxynaphthalene-4',6,8-trisu	220-036-2	2611-82-7	2611827	5803	Reach_1846	2926	604	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.3	-9.7	-11.3
2-[4-(4-ethoxyphenyl)-6-phenyl-1,3,5-triazin-2-yl]phenol	700-875-5	1195231-94-7	1195231947	1693	Reach_5017	2927	442	193.9	6.3E-07	1.6E+00	1.3E+03	11.6	9.51	3.5E-07	3.5E-08	1.1E-07				16%	-9.2	-9.7	-11.6
allyl 3-cyclohexylpropionate	220-292-5	2705-87-5	2705875	2493	Reach_1857	2928	196	17.3	2.9E+00	9.4E+01	3.0E+04			1.1E-06	3.5E-07	1.1E-06				17%	-9.9	-9.7	-11.1
7-anilino-4-hydroxynaphthalene-2-sulphonic acid	219-031-8	2321-07-5	2321075	1245	Reach_1784	2929	332	226.8	5.4E-12	2.5E+02	2.2E+03	9.01	0	1.1E-06	1.1E-07	3.5E-07				16%	-8.6	-9.7	-11.6
isobutyl 5-chloro-2,2-dimethylpentanoate	620-343-5	51336-94-8	51336948	3034	Reach_4566	2930	191	30.8	7.6E+00	4.5E+02	2.1E+02			1.1E-06	3.5E-07	1.1E-06				16%	-9.9	-9.7	-11.7
N-(2-ethylhexyl)naphthalen-2-amine	700-328-0	776-04-5	776045	3733	Reach_4862	2931	245	72.4	2.8E-01	7.6E+01	7.9E+03		0	3.5E-07	3.5E-08	1.1E-07				15%	-9.7	-9.7	-11.6
619-692-6	219-674-4	2495-37-6	2495376	565	Reach_1822	2932	176	11.8	4.5E+00	5.0E+02	9.5E+02	0	0	6.2E-07	1.1E-07	3.5E-07				15%	-8.9	-9.7	-11.5
dihexyl adipate	203-757-7	110-33-8	110338	1518	Reach_811	2933	314	-6.8	2.4E-02	8.6E-01	2.0E+06			1.1E-06	1.1E-07	3.5E-07				20%	-9.8	-9.7	-11.1
trifluoromethane	200-872-4	75-46-7	75467	3674	Reach_146	2934	70	-171.2	2.3E+06	2.1E+03	3.8E+00			3.5E-08	1.1E-08	3.5E-08				23%	-10.3	-9.7	-12.4
dibutyl 2,2'-thiobisacetate	223-914-3	4121-12-4	4121124	1264	Reach_2014	2935	262	3.1	1.9E-01	1.8E+02	8.9E+02			3.5E-06	3.5E-07	1.1E-06				14%	-9.9	-9.7	-11.6
3,3'-(1,4-Phenylene)bis(5,6-diphenyl-1,2,4-triazine)	258-221-5	52846-56-7	52846567	3078	Reach_2789	2936	382	275.5	2.1E-12	8.2E+01	4.0E+02			1.1E-06	3.5E-08	1.1E-07				21%	-9.1	-9.7	-11.0
N-{(1R)-1-cyano-2-[5-cyano-2-(trifluoromethyl)phenoxy]-1-met	600-753-0	106483-59-4	106483594	1436	Reach_4074	2937	367	235.2	4.4E-12	2.2E-01	1.4E+00	0.41		1.1E-06	1.1E-07	3.5E-07				18%	-8.9	-9.7	-11.3
605-546-9	209-080-3	555-06-6	555066	5932	Reach_1364	2938	159	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				16%	-9.9	-9.7	-11.5
1,3-Benzenediamine, coupled with diazotized m-phenylenediar	282-617-7	84281-74-3	84281743	3859	Reach_2970	2939	346	252.4	8.0E-11	3.5E+01	1.8E+02		8.88	1.1E-06	3.5E-07	1.1E-06				14%	-8.9	-9.7	-11.6
ethyl 2,3-epoxy-3-phenylbutyrate	201-061-8	77-83-8	77838	3738	Reach_186	2940	206	67.1	4.2E-01	6.6E+02	1.0E+03			1.1E-06	1.1E-07	3.5E-07				15%	-9.9	-9.7	-11.5
1,2,3,4-tetrahydroisoquinoline	202-050-0	91-21-4	91214	4014	Reach_373	2941	133	41.7	9.1E+00	7.1E+02	5.6E+01		5.1	3.5E-07	3.5E-08	1.1E-07				16%	-9.9	-9.7	-11.0
N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2,5-	235-426-8	12225-08-0	12225080	1744	Reach_2304	2942	577	349.8	8.7E-22	3.2E-02	3.2E+05	9.18	15.7	1.1E-06	1.1E-07	3.5E-07				14%	-9.1	-9.7	-11.6
hexanal	618-251-5	89182-60-5	89182605	3969	Reach_4489	2943	209	191.7	1.3E-09	9.7E+05	7.6E-05			3.5E-06	1.1E-06	3.5E-06				14%	-10.0	-9.7	-11.5
undecanal	203-972-6	112-44-7	112447	1589	Reach_907	2944	170	3.0	8.1E+00	1.3E+01	1.8E+04			3.5E-07	3.5E-08	1.1E-07				19%	-10.0	-9.7	-11.5
2-(2-heptadec-8-enyl-2-imidazolin-1-yl)ethanol	202-414-9	95-38-5	95385	4126	Reach_427	2945	351	175.5	3.1E-08	8.6E-02	3.2E+07	15.9	3.04	1.1E-06	3.5E-07	1.1E-06				22%	-9.1	-9.7	-10.6
tert-pentylbenzene	218-076-0	2049-95-8	2049958	2268	Reach_1751	2946	148	-16.4	7.0E+01	7.9E+00	2.5E+04			3.5E-07	3.5E-08	1.1E-07				22%	-10.0	-9.7	-12.2
cyclopentylamine	213-697-3	1003-03-8	1003038	1298	Reach_1632	2947	85	-38.2	3.5E+03	4.1E+04	1.4E+01		3.5	1.1E-06	3.5E-07	3.5E-07				15%	-9.9	-9.7	-11.1
1-o-tolylbiguanide	202-268-6	93-69-6	93696	4079	Reach_406	2948	191	136.3	4.9E-04	1.8E+03	1.1E+01		3	3.5E-06	1.1E-07	3.5E-07				14%	-8.7	-9.7	-11.8
2-methylaziridine	200-878-7	75-55-8	75558	3676	Reach_150	2949	57	-50.9	2.0E+04	7.8E+05	1.3E+00		5.5	3.5E-06	1.1E-06	3.5E-06				14%	-9.9	-9.7	-11.2
N-(3-{[5-(4-chlorophenyl)-1-(2,6-dichlorobenzoyl)-1H-pyrrolo[2	700-829-4	5324-06-1	5324061	1273	Reach_5003	2950	212	117.0	4.8E-06	3.5E+04	8.1E-02	14	0	3.5E-06	1.1E-06	3.5E-06				19%	-9.5	-9.7	-11.3
trifluoromethanesulphonic acid	216-087-5	1493-13-6	1493136	2005	Reach_1687	2951	150	23.9	7.3E+01	2.7E+04	3.2E-01	-2.76		3.5E-06	1.1E-06	3.5E-06				14%	-8.7	-9.7	-11.6
dimethoxydimethylsilane	214-189-4	1112-39-6	1112396	1544	Reach_1647	2952	120	-78.5	1.1E+04	4.7E+03	3.8E+00			1.1E-06	3.5E-07	1.1E-06				17%	-10.0	-9.7	-12.1
methyl 3-α,7-α-diacetoxy-12-oxo-5-β-cholan-24-oate	615-497-5	71809-65-9	71809659	6010	Reach_4415	2953	225	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				20%	-9.1	-9.7	-11.2
[nitrilotris(methylene)]trisphosphonic acid, potassium salt	279-900-2	82104-74-3	82104743	3817	Reach_2962	2954	159	92.5	1.2E-02	2.8E+03	1.8E+00									18%	-9.4	-9.7	-11.4
diisopropyl adipate	230-072-0	6938-94-9	6938949	3541	Reach_2213	2955	230	-48.3	5.9E+00	4.9E+02	1.6E+03			3.5E-06	3.5E-07	1.1E-06				14%	-10.0	-9.7	-11.4
4,4'-cyclohexylidenedi-o-cresol	237-163-4	13676-54-5	13676545	1901	Reach_2344	2956	358	298.3	5.5E-14	1.0E+02	6.3E+01	0		1.1E-06	1.1E-07	3.5E-07				20%	-9.3	-9.7	-11.2
Potassium (2S)-4-carboxy-2-(tetradecanoylamino)butanoate	700-277-4	2827-56-7	2827567	5816	Reach_4837	2957	152	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.4	-9.7	-11.4
N4-[3-(1H-imidazol-1-yl)propyl]-2-methylbenzene-1,4-diamine	700-408-5	103429-90-9	103429909	1366	Reach_4890	2958	160	-20.1	2.0E+02	3.5E+03	2.9E+01									18%	-9.4	-9.7	-11.4
11-piperazin-1-yldibenzo[b,f][1,4]thiazepine dihydrochloride	700-144-0	13115-71-4	13115714	1846	Reach_4780	2959	203	308.1	1.6E-09	3.4E+04	6.6E-04									18%	-9.4	-9.7	-11.4
sec-butyl chloroformate	620-313-1	877179-03-8	877179038	3938	Reach_4564	2960	298	184.1	2.7E-06	2.4E+00	6.2E+03			3.5E-07	1.1E-08	3.5E-08				15%	-10.0	-9.7	-12.1
1-ethyl-1H-imidazol-3-ium trifluoromethanesulfonate	700-183-3	52299-25-9	52299259	3057	Reach_4796	2961	502	10.4	3.9E+01	2.9E-04	1.9E+04									18%	-9.4	-9.7	-11.4
3-amino-4-methoxybenzanilide	204-388-4	120-35-4	120354	1710	Reach_992	2962	242	186.8	1.8E-06	4.8E+01	7.2E+01	15	10.7	1.1E-06	3.5E-07	1.1E-06				14%	-9.0	-9.7	-11.6
calcium dilactate	700-276-9	111974-74-4	111974744	5609	Reach_4836	2963	332	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.4	-9.7	-11.4
(3-aminophenyl)uronium chloride	700-345-3	515851-08-8	515851088	5907	Reach_4870	2964	340	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.4	-9.7	-11.4
1,1,3,3-tetramethyl-1,3-divinyldisiloxane	220-099-6	2627-95-4	2627954	2462	Reach_1849	2965	186	-56.9	6.0E+04		9.1E+05			1.1E-06	1.1E-07	3.5E-07				22%	-10.0	-9.7	-12.7
Sodium 4-fluorobenzene sulfinate	806-798-4	1262985-23-8	1262985238	1803	Reach_5081	2966	663	333.5	1.8E-16	1.9E-05	1.0E+07									18%	-9.4	-9.7	-11.4
1-aminoimidazolidine-2,4-dione hydrochloride	700-027-4	17247-58-4	17247584	2127	Reach_4730	2967	149	-44.9	1.5E+03	2.1E+02	8.9E+02									18%	-9.4	-9.7	-11.4
1,3-propanesultone	214-317-9	1120-71-4	1120714	1572	Reach_1660	2968	122	25.5	3.2E+01	1.4E+05	5.2E-01			1.1E-05	1.1E-06	3.5E-06				14%	-9.9	-9.7	-11.7
605-260-4	605-260-4	161599-46-8	161599468	2080	Reach_4171	2969	329	150.5	3.6E-05	5.0E+02	4.3E-01		12	3.5E-06	3.5E-07	1.1E-06				14%	-8.6	-9.7	-11.7
1-[1,6-dimethyl-4-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]eth	260-772-1	57499-57-7	57499577	3231	Reach_2825	2970	234	65.5	1.8E-01	4.2E+00	3.4E+05			1.1E-06	3.5E-07	1.1E-06				19%	-9.9	-9.7	-11.2
N-(5-chloro-2-methoxyphenyl)-2-[(2-methoxy-4-nitrophenyl)az	240-131-2	15993-42-7	15993427	2069	Reach_2407	2971	421	250.3	1.1E-10	1.3E+00	4.3E+03	8.66	15.1	3.5E-07	3.5E-08	1.1E-07				16%	-9.2	-9.7	-11.6
2-methylbutyric acid	612-179-8	61597-98-6	61597986	3340	Reach_4372	2972	228	47.7	1.3E-02	3.2E+01	2.2E+03	12.6		3.5E-06	3.5E-07	1.1E-06				14%	-9.5	-9.7	-11.7
6-hydroxy-2-naphthoic acid	240-759-7	16712-64-4	16712644	2111	Reach_2428	2973	188	141.0	7.3E-05	4.5E+02	3.7E+02	4.55		3.5E-06	1.1E-07	3.5E-07				14%	-9.0	-9.7	-11.8
amitriptyline	226-971-2	5580-58-5	5580585	3179	Reach_2127	2974	957	349.8	1.1E-28	3.2E-10	5.6E+07		10.9	3.5E-09	3.5E-09	3.5E-09				23%	-9.7	-9.7	-10.8
2-(1-methylethoxy)ethyl acetate	242-901-3	19234-20-9	19234209	2228	Reach_2476	2975	146	-38.2	3.7E+02	1.6E+04	1.0E+01			1.1E-06	3.5E-07	1.1E-06				14%	-10.0	-9.7	-11.2
ethylene dimethacrylate	202-617-2	97-90-5	97905	4175	Reach_491	2976	198	-68.4	1.1E+04	2.0E+03	1.6E+02			3.5E-06	3.5E-07	1.1E-06				17%	-10.0	-9.7	-12.7
3-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexan-1-ol	254-384-1	39255-32-8	39255328	2837	Reach_2724	2977	144	-43.9	3.8E+02	1.4E+03	5.8E+02	0		3.5E-06	3.5E-07	1.1E-06				18%	-9.7	-9.7	-11.4

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
2-chloro-N-mesitylacetamide	202-892-9	100-83-4	100834	138	Reach_570	2978	122	42.6	4.0E-01	8.2E+03	1.7E+01	9.1	0	1.4E-06	1.1E-06	3.5E-06				16%	-8.9	-9.7	-11.6
methyl 3,3-dimethylpent-4-enoate	264-431-8	63721-05-1	63721051	3417	Reach_2862	2979	142	-39.1	6.2E+02	3.4E+03	3.8E+02			3.5E-06	3.5E-07	1.1E-06				14%	-10.0	-9.7	-11.6
dichloro(3-chloropropyl)methylsilane	232-136-3	7787-93-1	7787931	3741	Reach_2276	2980	192	-31.3	3.8E+02	8.1E+02	3.0E+03			1.1E-07	1.1E-08	3.5E-08				21%	-10.0	-9.7	-11.6
2-methylundecanal	203-765-0	110-41-8	110418	1519	Reach_812	2981	184	3.2	2.0E+02	2.9E+00	4.7E+04			3.5E-07	3.5E-08	1.1E-07				22%	-10.0	-9.7	-12.5
5,7-Dimethoxy[1,2,4]triazolo[1,5-a]pyrimidin-2-amine	603-562-0	13223-43-3	13223433	1856	Reach_4124	2982	195	141.2	1.4E-03	6.2E+04	1.9E+01		9.4	1.1E-06	1.1E-07	1.1E-06				14%	-9.0	-9.7	-11.7
2-[(E)-(2-methoxy-5-nitrophenyl)diazenyl]-N-(2-methoxypheny	228-788-3	6358-87-8	6358878	3411	Reach_2172	2983	740	349.8	5.4E-21	4.0E-06	1.7E+09	0	0	3.5E-07	3.5E-08	3.5E-08				16%	-8.9	-9.7	-11.5
2-ethoxy-6-hydroxypyrimidin-4(1H)-one	692-762-1	166524-65-8	166524658	2105	Reach_4679	2984	160	19.5	1.2E+02	3.0E+03	6.5E+01	0		1.1E-06	1.1E-07	1.1E-06				14%	-8.4	-9.7	-11.8
1-phenylethyl acetate	616-466-9	77501-63-4	77501634	882	Reach_4440	2985	462	178.0	2.6E-05	7.9E-02	8.3E+04			1.4E-07	1.1E-07	3.5E-07				15%	-10.0	-9.7	-11.2
D-α-methylbenzylamine	618-153-2	88374-05-4	88374054	3955	Reach_4488	2986	232	78.5	1.2E-01	3.5E+01	4.6E+03		0	1.1E-06	1.1E-07	3.5E-07				16%	-10.0	-9.7	-11.1
L-α-methylbenzylamine	639-778-7	887148-70-1	887148701	3963	Reach_4606	2987	473	240.1	5.5E-10	1.8E-02	1.3E+05		0	1.1E-06	1.1E-07	3.5E-07				16%	-10.0	-9.7	-11.1
2-amino-5-bromopyridin-3-ol	601-411-3	116091-63-5	116091635	1643	Reach_4087	2988	243	144.1	2.0E-04	1.7E+04	8.5E-01	9.87	0	1.1E-06	1.1E-07	3.5E-07				16%	-8.8	-9.7	-11.6
3,3'-iminodi(propylamine)	610-954-5	53075-09-5	53075095	5919	Reach_4341	2989	211	0.0	0.0E+00	0.0E+00	0.0E+00		0	0.0E+00	0.0E+00	0.0E+00				14%	-9.3	-9.7	-11.9
ethyl 2-methyl-1,3-dioxolane-2-acetate	218-145-5	2052-25-7	2052257	5769	Reach_1754	2990	382	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				14%	-10.0	-9.7	-11.7
androstanolone	700-599-5	54761-87-4	54761874	690	Reach_4946	2991	306	206.8	9.0E-08	1.3E+02	2.3E+01	0		5.7E-08	1.1E-07	3.5E-07				18%	-9.3	-9.7	-11.4
5-nitrofurfurylidene di(acetate)	202-166-1	92-55-7	92557	4040	Reach_387	2992	243	66.8	4.8E-02	2.5E+03	5.5E+00			3.5E-06	3.5E-07	1.1E-06				14%	-9.6	-9.7	-11.8
2,2-dimethyl-1,3-dioxane-4,6-dione	217-992-8	2033-24-1	2033241	2261	Reach_1747	2993	144	26.7	4.4E-02	6.7E+04	6.2E+04	5.1		3.5E-06	3.5E-07	1.1E-06				14%	-9.0	-9.7	-11.6
618-153-2	940-185-3	32860-09-6	32860096	2664	Reach_5166	2994	248	172.0	2.7E-07	2.8E+02	4.4E+01			1.1E-06	3.5E-07	1.1E-06				15%	-10.0	-9.7	-11.5
N-methyl-1-(methylthio)-2-nitrovinylamine	619-739-0	874208-98-7	874208987	3933	Reach_4540	2995	200	26.2	2.8E+00	3.4E+02	1.5E+02		0	3.5E-06	3.5E-07	1.1E-06				16%	-9.5	-9.7	-11.6
3-nitro-p-toluic acid	612-185-0	61636-08-6	61636086	3344	Reach_4374	2996	156	175.7	5.5E-08	1.6E+03	6.9E-02	4.6		3.5E-06	3.5E-07	1.1E-06				14%	-9.0	-9.7	-11.8
619-997-4	617-385-1	82784-24-5	82784245	6045	Reach_4459	2997	638	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				16%	-9.0	-9.7	-11.6
8-benzyl-8-azabicyclo[3.2.1]octan-3-one oxime	607-884-2	261953-36-0	261953360	2458	Reach_4251	2998	246	109.6	2.3E-02	4.5E+02	2.3E+02	0	7.2	1.1E-06	1.1E-07	3.5E-07				16%	-8.9	-9.7	-11.6
1-(allyloxy)-2-methyl-1-oxopropan-2-yl 5-amino-2-chlorobenzo	696-318-8	174489-43-1	174489431	2137	Reach_4714	2999	298	96.5	1.7E-03	5.0E+01	1.6E+03		11.3	1.1E-06	1.1E-07	3.5E-07				14%	-9.2	-9.7	-11.8
(hydroxyethyl)urea	215-304-0	1320-51-0	1320510	1853	Reach_1676	3000	104	57.4	2.0E-01	1.1E+05	7.2E-03	13.3	14.7	3.5E-06	3.5E-07	1.1E-06				14%	-8.5	-9.7	-11.8
o-(1-methylheptyl)phenol	242-459-1	18626-98-7	18626987	2201	Reach_2466	3001	206	80.2	2.3E-02	1.0E+00	2.6E+05	10.8		3.5E-07	3.5E-08	1.1E-07				20%	-10.0	-9.8	-11.0
methyl (3-hydroxyphenyl)-carbamate	207-434-1	471-01-2	471012	2962	Reach_1288	3002	138	17.4	6.4E+01	6.1E+02	2.1E+02	0		1.1E-06	3.5E-07	1.1E-06				14%	-9.2	-9.8	-11.9
4,4'-oxydianiline	202-977-0	101-80-4	101804	1329	Reach_583	3003	200	130.5	3.4E-04	3.2E+03	1.7E+02		8.62	1.1E-06	1.1E-07	3.5E-07				14%	-9.0	-9.8	-11.7
dimethyl (2-acetoxyethyl)phosphonate	604-710-7	149934-21-4	149934214	5708	Reach_4160	3004	509	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				14%	-9.8	-9.8	-11.9
trans-N,N,N',N'-Tetrakis(2-hydroxyethyl)cyclohexane-1,4-dicar	243-848-9	20485-39-6	20485396	2266	Reach_2494	3005	155	32.0	2.3E+01	3.9E+03	6.9E+00	0	14.9	3.5E-06	3.5E-07	1.1E-06				14%	-8.4	-9.8	-11.8
606-114-2	255-980-4	42872-29-7	42872297	2901	Reach_2752	3006	194	82.4	4.6E-02	3.1E+02	2.6E+01			3.5E-07	1.1E-07	3.5E-07				17%	-10.0	-9.8	-11.1
1-bromo-2-methylpropane	619-905-2	915416-45-4	915416454	4018	Reach_4553	3007	223	94.2	2.2E-02	4.7E+01	2.8E+03			3.5E-06	1.1E-07	3.5E-07				17%	-10.1	-9.8	-12.7
N-ethylpropylamine	243-573-4	20193-20-8	20193208	2253	Reach_2489	3008	87	-66.9	1.1E+04	1.8E+05	2.0E+01		3.1	1.1E-05	3.5E-07	1.1E-06				14%	-10.0	-9.8	-11.5
2,5-di-tert-pentylhydroquinone	201-222-2	79-74-3	79743	3781	Reach_248	3009	250	124.9	3.8E-05	2.5E+01	6.8E+05	10.1		1.1E-06	1.1E-07	3.5E-07				19%	-9.3	-9.8	-11.3
1,1',1''-[methylidynetris(oxy)]trispropane	210-704-1	621-76-1	621761	3363	Reach_1443	3010	190	-3.4	1.1E+02	5.2E+05	8.3E+02			1.1E-06	3.5E-07	1.1E-06				15%	-10.0	-9.8	-11.6
iodotrimethylsilane	240-171-0	16029-98-4	16029984	2073	Reach_2408	3011	200	-65.9	2.9E+03	6.9E+02	9.8E+02			3.5E-09	3.5E-09	3.5E-09				24%	-10.3	-9.8	-12.3
(pentabromophenyl)methyl acrylate	261-767-7	59447-55-1	59447551	3278	Reach_2836	3012	557	171.4	1.8E-05	1.6E-03	7.8E+06			3.5E-06	3.5E-07	1.1E-06				20%	-9.8	-9.8	-11.4
ammonium difluoro[1,1,2,2-tetrafluoro-2-(pentafluoroethoxy)e	610-992-2	53378-52-2	53378522	5921	Reach_4344	3013	248	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.5	-9.8	-11.4
ethyl 3-[[bis(1-methylethoxy)phosphinothioyl]thio]propionate	275-965-6	71735-74-5	71735745	3588	Reach_2930	3014	314	17.0	2.1E-02	7.0E+00	1.4E+04			3.5E-06	3.5E-07	1.1E-06				15%	-10.0	-9.8	-11.6
Sodium O,O-diisobutyl phosphorothioate	700-323-3	908020-52-0	908020520	6080	Reach_4860	3015	363	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.5	-9.8	-11.4
N'-(3-aminopropyl)-N,N-dimethylpropane-1,3-diamine	234-148-4	10563-29-8	10563298	1418	Reach_2298	3016	159	40.4	5.8E+00	1.0E+06	3.4E-01		3.57	3.5E-06	3.5E-07	1.1E-06				14%	-9.2	-9.8	-11.9
pentobarbital	700-355-8	42036-65-7	42036657	5884	Reach_4873	3017	192	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				16%	-9.1	-9.8	-11.5
1,2,3,5,6,7-hexahydro-1,1,2,3,3-pentamethyl-4H-inden-4-one	251-649-3	33704-61-9	33704619	2684	Reach_2669	3018	206	70.8	5.4E-01	6.2E+01	3.1E+04			1.1E-06	3.5E-07	1.1E-06				16%	-10.0	-9.8	-11.3
tert-butyl [2-({[1-methyl-5-(tritylamino)-1H-pyrazol-4-yl]carban	200-350-6	57-83-0	57830	65	Reach_43	3019	314	149.8	3.6E-04	4.0E+01	4.7E+03	0	0	3.4E-07	3.5E-08	1.1E-07				16%	-9.4	-9.8	-11.6
tris(p-isocyanatophenyl) thiophosphate	223-981-9	4151-51-3	4151513	2880	Reach_2016	3020	465	90.3	2.7E-06	2.7E-02	1.9E+08			1.1E-06	3.5E-07	1.1E-06				23%	-9.2	-9.8	-10.5
N-[3-(dimethylamino)propyl]acrylamide	619-422-7	99305-42-7	99305427	4202	Reach_4520	3021	88	-88.1	1.9E+04	2.1E+04	3.5E+01	0	0	1.1E-06	1.1E-07	3.5E-07				14%	-9.1	-9.8	-11.9
flucytosine	204-522-1	122-09-8	122098	1742	Reach_1026	3022	149	29.0	3.2E+01	1.4E+01	1.6E+02	0	4.1	3.5E-07	3.5E-08	1.1E-07				16%	-8.8	-9.8	-11.7
2-methoxyethyl cyanoacetate	611-267-3	554-52-9	554529	3170	Reach_4355	3023	167	86.1	3.6E-02	3.8E+03	4.8E+00			3.5E-06	3.5E-07	1.1E-06				14%	-10.0	-9.8	-11.8
3-(dodecylamino)propiononitrile	606-114-2	187592-70-7	187592707	2207	Reach_4194	3024	277	58.2	5.8E-01	4.3E+01	1.7E+03		0	3.5E-07	1.1E-07	3.5E-07				17%	-10.0	-9.8	-11.5
3-dimethylaminopropan-1-ol	226-970-7	5580-57-4	5580574	3178	Reach_2126	3025	937	349.8	1.7E-28	6.7E-10	4.5E+07	8.41	9.13	3.5E-08	1.1E-08	1.1E-08				14%	-9.9	-9.8	-11.8
1,1-dimethylprop-3-ynylamine	221-029-7	2978-58-7	2978587	2571	Reach_1893	3026	83	-25.9	1.2E+04	6.0E+05	2.8E+00		6	3.5E-06	3.5E-07	1.1E-06				14%	-10.0	-9.8	-11.4
cyclopropyl methyl ketone	212-146-4	765-43-5	765435	3717	Reach_1540	3027	84	-57.5	3.6E+03	3.1E+04	3.6E+00			1.1E-06	3.5E-07	1.1E-06				15%	-10.0	-9.8	-11.2
609-205-5	251-347-1	33021-02-2	33021022	2673	Reach_2667	3028	130	-67.5	4.4E+03	1.4E+02	6.8E+02			1.1E-06	3.5E-07	1.1E-06				18%	-9.9	-9.8	-11.5
vinyl neononanoate	259-160-7	54423-67-5	54423675	3143	Reach_2798	3029	184	-4.0	3.0E+01	6.3E+01	1.1E+04			3.5E-06	3.5E-07	1.1E-06				16%	-10.1	-9.8	-11.9
decyloxirane	220-667-3	2855-19-8	2855198	2537	Reach_1876	3030	184	9.4	1.4E+01	4.7E+00	6.2E+04			3.5E-07	3.5E-08	1.1E-07				22%	-10.1	-9.8	-12.1
oxolamine	207-096-5	434-03-7	434037	2911	Reach_1272	3031	312	168.6	3.2E-08	5.8E+00	2.8E+03		0	3.5E-07	3.5E-08	1.1E-07				16%	-9.8	-9.8	-11.6
2-methylcyclohexyl acetate	227-231-1	5726-19-2	5726192	3228	Reach_2133	3032	156	-18.5	6.5E+01	1.8E+03	1.1E+03			3.5E-06	3.5E-07	1.1E-06				14%	-10.0	-9.8	-11.4
N,N'-ethylenedi(diacetamide)	700-469-8	187666-88-2	187666882	2208	Reach_4904	3033	186	197.3	3.7E-07	1.4E+04	3.3E+00	5.3	0	1.1E-06	3.5E-07	1.1E-06				14%	-8.5	-9.8	-11.8
2-[ethyl(4-nitrosophenyl)amino]ethyl [3-(triethoxysilyl)propyl]c	700-840-4	160583-22-2	160583222	2075	Reach_5006	3034	201	72.5	2.7E-02	3.4E+02	1.3E+03	0	0	1.1E-06	1.1E-07	3.5E-07				16%	-9.3	-9.8	-11.7
N,N-dimethylhydrazine	200-316-0	57-14-7	57147	720	Reach_40	3035	60	-61.3	2.2E+04	6.4E+05	6.5E-02		6	7.3E-09	1.1E-07	3.5E-07				23%	-10.1	-9.8	-10.8
tert-butyl acetate	208-760-7	540-88-5	540885	684	Reach_1336	3036	116	-62.5	5.7E+03	4.9E+03	5.5E+01			1.9E-07	3.5E-07	1.1E-06				20%	-10.1	-9.8	-11.8
chlorodiphenylphosphine	225-059-1	4635-59-0	4635590	2951	Reach_2050	3037	141	-22.2	1.8E+02	4.0E+02	5.8E+00			3.5E-08	1.1E-08	1.1E-08				16%	-10.1	-9.8	-11.3
1,1,3-trichloroacetone	203-963-7	112-36-7	112367	327	Reach_901	3038	162	-15.2	1.2E+02	4.6E+05	3.2E+00			9.8E-07	1.1E-07	3.5E-07				20%	-10.1	-9.8	-11.5
2-{[(4-chloro-3-methylpyridin-2-yl)methyl]thio}-1H-benzimidaz	600-066-6	1003315-69-2	1003315692	1300	Reach_4055	3039	349	191.4	9.1E-07	1.2E-01	6.9E+04	0	0	1.1E-06	1.1E-07	3.5E-07				16%	-9.3	-9.8	-11.6
606-239-2	262-540-5	60958-45-4	60958454	5948	Reach_2848	3040	508	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				14%	-8.7	-9.8	-11.8
(+)-pin-2(3)-ene	232-087-8	7785-70-8	7785708	888	Reach_2274	3041	136	-13.6	5.4E+02	2.8E+01	1.9E+04			9.7E-08	3.5E-08	1.1E-07				23%	-10.1	-9.8	-12.4
2-[(4-methyl-2-nitrophenyl)azo]-3-oxo-N-phenylbutyramide	219-730-8	2512-29-0	2512290	2416	Reach_1825	3042	340	224.9	5.7E-09	5.3E+00	8.7E+03	8.62	13.7	3.5E-06	3.5E-08	1.1E-07				15%	-8.9	-9.8	-11.7
methyl 2-oxopyrrolidin-1-acetate	261-926-0	59776-88-4	59776884	3287	Reach_2842	3043	157	69.9	3.1E-01	1.3E+05	8.5E-01		15.8	3.5E-06	3.5E-07	1.1E-06				14%	-8.6	-9.8	-11.8
2-{(R)-[(3-Methyl-4-nitropyridin-2-yl)methyl]sulfinyl}-1H-benzir	700-088-7	6764-10-9	6764109	1285	Reach_4757	3044	266	139.8	2.6E-04	2.8E+00	5.6E+04			3.5E-08	1.1E-08	3.5E-08				18%	-9.5	-9.8	-11.5
sodium 4-aminonaphthalene-1-sulphonate	200-574-4	64-04-0	64040	3423	Reach_69	3045	121	10.9	5.5E+01	1.2E+03	2.2E+01									18%	-9.5	-9.8	-11.5
dipotassium dihydrogen ethylenediaminetetraacetate	217-895-0	2001-94-7	2001947	5765	Reach_1743	3046	368	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.5	-9.8	-11.5
tert-butyl 4-(6-nitropyridin-3-yl)piperazine-1-carboxylate	691-244-2	106939-34-8	106939348	1450	Reach_4666	3047	309	146.2	1.9E-04	7.0E+00	9.5E+00		15.2	1.1E-06	1.1E-07	3.5E-07				16%	-9.1	-9.8	-11.6
3,5,5-trimethylhexyl acetate	261-245-9	58430-94-7	58430947	3247	Reach_2829	3048	186	-13.6	5.1E+01	1.5E+01	1.3E+04			3.5E-06	3.5E-07	1.1E-06				17%	-10.1	-9.8	-12.6
619-738-5	207-925-0	501-53-1	501531	653	Reach_1299	3049	171	11.6	4.9E+02	7.7E+02	6.9E+01			6.4E-07	3.5E-07	1.1E-06				14%	-10.0	-9.8	-11.7
616-210-6	604-437-3	144690-92-6	144690926	1979	Reach_4153	3050	801	349.8	1.7E-32	2.2E-11	7.1E+08			3.5E-07	3.5E-08	1.1E-07				19%	-9.2	-9.8	-11.4
2-(4-fluorophenyl)-5-(5-iodo-2-methylbenzyl)thiophene	618-312-6	898566-17-1	898566171	3987	Reach_4494	3051	408	174.0	2.6E-06	9.4E-03	5.6E+07			1.1E-06	1.1E-07	3.5E-07				22%	-9.3	-9.8	-10.8
2-methylbutyraldehyde	203-336-8	105-83-9	105839	1420	Reach_651	3052	145	45.3	5.7E+00	3.8E+05	1.1E-01			3.5E-06	1.1E-07	1.1E-06				15%	-10.1	-9.8	-11.1

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
dibutyl methylenedithiodi(acetate)	238-289-2	14338-82-0	14338820	1965	Reach_2363	3053	308	4.4	1.3E-02	2.0E+01	6.8E+03			3.5E-06	3.5E-07	1.1E-06				15%	-10.1	-9.8	-11.7
dichloro(diphenyl)silane	201-251-0	80-10-4	80104	3788	Reach_258	3054	253	66.9	8.1E-02	1.1E+01	1.1E+05			1.1E-06	1.1E-07	3.5E-07				18%	-10.0	-9.8	-11.4
612-179-8	204-145-2	116-53-0	116530	1650	Reach_955	3055	102	3.6	1.5E+02	3.7E+04	3.1E+01	4.9		3.5E-06	3.5E-07	1.1E-06				14%	-10.1	-9.8	-11.7
(S)-2,2,3-trimethylcyclopent-3-ene-1-acetaldehyde	245-846-3	23727-15-3	23727153	2356	Reach_2533	3056	152	11.5	3.2E+01	5.2E+02	2.0E+03			1.1E-06	3.5E-07	1.1E-06				15%	-10.1	-9.8	-11.3
609-206-0	608-291-1	2890-61-1	2890611	2548	Reach_4269	3057	161	8.5	9.5E+01	6.2E+01	1.8E+02			3.5E-07	1.1E-07	3.5E-07				19%	-9.9	-9.8	-11.5
617-648-0	617-648-0	849727-62-4	849727624	6056	Reach_4470	3058	275	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.5	-9.8	-11.5
carbonohydrazide	207-837-2	497-18-7	497187	2989	Reach_1296	3059	90	77.9	1.4E-01	1.0E+06	1.9E-04	14.3	9.9	3.5E-06	1.1E-06	3.5E-06				14%	-8.7	-9.8	-11.8
N-(5-chloro-2-methylphenyl)-3-hydroxy-4-[[2-methoxy-5-[(phe	610-868-8	52603-48-2	52603482	3065	Reach_4337	3060	163	118.4	3.6E-03	1.8E+03	1.2E+01	0	0	1.1E-06	1.1E-07	3.5E-07				19%	-9.6	-9.8	-11.4
3-(trimethoxysilyl)propyl (2E,4E)-hexa-2,4-dienoate	642-902-2	163802-53-7	163802537	2089	Reach_4611	3061	274	62.0	8.2E-02	1.7E+02	2.5E+01			3.5E-06	3.5E-07	1.1E-06				14%	-10.1	-9.8	-11.8
Diphenylmethyl (6R,7R)-3-hydroxy-8-oxo-7-[(phenylacetyl)amir	611-177-4	54639-48-4	54639484	3150	Reach_4351	3062	501	328.2	1.3E-19	8.0E-01	3.8E+02	9.45		3.5E-07	3.5E-08	1.1E-07				16%	-9.0	-9.8	-11.6
615-309-1	270-027-2	68400-38-4	68400384	5996	Reach_2905	3063	658	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-9.2	-9.8	-11.9
4-isopropylbenzaldehyde	616-309-4	762240-92-6	762240926	6031	Reach_4432	3064	229	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				15%	-10.1	-9.8	-11.2
2-chloro-3-(2-chloroethyl)-1,3,2-oxazaphosphinane 2-oxide	692-156-7	1101184-94-4	1101184944	5605	Reach_4673	3065	243	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				16%	-9.9	-9.8	-11.7
benzyl [(2S)-1-[(2-aminoethyl)amino]-3-(4-ethoxyphenyl)propa	617-838-3	86357-14-4	86357144	3905	Reach_4475	3066	381	304.9	1.9E-14	1.4E+04	1.6E-01									18%	-9.5	-9.8	-11.5
dimethyl 3-oxoglutarate	692-944-0	1363332-77-7	1363332777	5679	Reach_4683	3067	407	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-10.0	-9.8	-11.9
1,2,3,6,-tetrahydro-N-(2-hydroxyethyl)phthalimide	605-546-9	169280-10-8	169280108	2116	Reach_4179	3068	260	106.7	4.4E-03	2.1E+00	8.3E+03	0	0	1.1E-06	1.1E-07	3.5E-07				14%	-8.6	-9.8	-11.8
617-347-4	617-347-4	82543-16-6	82543166	3829	Reach_4455	3069	330	180.1	2.9E-08	6.0E+02	2.7E+02	15.4		3.5E-07	3.5E-08	1.1E-07				16%	-8.9	-9.8	-11.6
glutaric anhydride	203-593-6	108-55-4	108554	1485	Reach_748	3070	114	-42.1	2.7E-01	5.0E+04	2.0E+01			3.5E-06	3.5E-07	1.1E-06				14%	-9.3	-9.8	-11.8
4-(2-aminoethyl)-2-methoxyphenol	233-597-3	10258-54-5	10258545	1346	Reach_2286	3071	129	6.2	2.7E+01	4.3E+04	4.3E-02	0	0	3.5E-06	3.5E-07	1.1E-06				14%	-9.4	-9.8	-11.8
chlorotrifluoroethylene	201-201-8	79-38-9	79389	3774	Reach_243	3072	116	-135.7	5.6E+05	6.8E+01	4.5E+01			3.5E-08	1.1E-08	1.1E-08				23%	-10.3	-9.8	-12.6
2-cyano-N-[(ethylamino)carbonyl]acetamide	255-202-3	41078-06-2	41078062	2869	Reach_2734	3073	155	171.0	1.9E-05	3.9E+04	1.6E+00	7.11	15.1	1.1E-06	3.5E-07	1.1E-06				14%	-8.7	-9.8	-11.8
604-481-3	700-279-5	4707-49-7	4707497	2961	Reach_4838	3074	168	138.6	1.0E-04	1.6E+04	2.0E+02			3.5E-06	3.5E-07	1.1E-06				15%	-10.1	-9.8	-11.4
dimethyl cyclohexane-1,4-dicarboxylate	202-347-5	94-60-0	94600	4106	Reach_416	3075	200	-46.4	1.1E+01	8.9E+03	1.3E+02			3.5E-06	3.5E-07	1.1E-06				14%	-10.1	-9.8	-11.7
p-menth-1-en-8-yl acetate	203-689-8	109-63-7	109637	1505	Reach_781	3076	142	0.0	0.0E+00	0.0E+00	0.0E+00			1.1E-06	3.5E-07	1.1E-06				17%	-10.1	-9.8	-11.3
608-177-1	608-177-1	282102-50-5	282102505	5815	Reach_4263	3077	470	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.5	-9.8	-11.5
2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-eth	208-797-9	542-05-2	542052	3134	Reach_1344	3078	146	117.3	5.5E-03	1.8E+05	4.9E-03	3.19	0	3.5E-06	3.5E-07	1.1E-06				16%	-9.5	-9.8	-11.7
[1α(E),2β]-1-(2,6,6-trimethylcyclohex-3-en-1-yl)but-2-en-1-one	275-156-8	71048-82-3	71048823	3577	Reach_2925	3079	192	33.7	3.6E+00	6.9E+01	1.4E+04			1.1E-06	3.5E-07	1.1E-06				16%	-10.1	-9.8	-11.3
hexyl laurate	251-932-1	34316-64-8	34316648	2700	Reach_2675	3080	284	72.5	1.3E-02	3.4E-02	5.5E+07			1.1E-06	1.1E-07	3.5E-07				22%	-9.8	-9.8	-11.5
17α-hydroxy-2-(hydroxymethylene)pregn-4-en-20-yn-3-one	600-715-3	106092-09-5	106092095	1428	Reach_4072	3081	169	113.7	1.3E-02	8.2E+04	7.8E+00	0		3.5E-06	3.5E-07	1.1E-06				16%	-9.2	-9.8	-11.7
609-521-3	609-205-5	361366-15-6	361366156	2758	Reach_4293	3082	318	93.5	1.2E-03	2.5E+00	3.2E+05		0	1.1E-06	1.1E-07	3.5E-07				14%	-8.8	-9.8	-11.9
methyl cinnamate	203-093-8	103-26-4	103264	1362	Reach_605	3083	162	9.7	1.7E+00	3.7E+02	2.3E+02			3.5E-06	3.5E-07	1.1E-06				14%	-10.1	-9.8	-11.7
strontium bis[2-chloro-5-[(2-hydroxy-1-naphthyl)azo]toluene-4	277-335-6	73263-40-8	73263408	6013	Reach_2938	3084	839	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.5	-9.8	-11.5
2-amino-6-{[(3S)-1-(3-methylbutanoyl)piperidin-3-yl]methoxy}t	700-511-5	1917-64-2	1917642	2225	Reach_4916	3085	140	17.7	3.3E+01	6.3E+04	4.1E+00		0	3.5E-06	1.1E-06	3.5E-06				16%	-9.4	-9.8	-11.7
ethyl 2-oxopyrrolidine-1-acetate	205-532-9	142-29-0	142290	1952	Reach_1176	3086	68	-93.2	5.1E+04	8.9E+02	3.0E+02		0	1.1E-06	1.1E-07	3.5E-07				14%	-8.7	-9.8	-11.8
triethoxy(methyl)silane	255-255-2	41198-08-7	41198087	631	Reach_2738	3087	374	86.5	1.0E-03	4.1E-01	6.6E+04			3.9E-09	1.1E-07	3.5E-07				16%	-10.1	-9.8	-11.9
nonamethylenediamine	211-470-3	646-24-2	646242	3439	Reach_1483	3088	158	49.2	2.3E+00	1.3E+03	6.6E+01		3.2	3.5E-07	1.1E-07	3.5E-07				16%	-10.1	-9.9	-11.5
3-(hydroxymethyl)pyridinium fluoride	700-352-1	62756-44-9	62756449	5958	Reach_4872	3089	129	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.6	-9.9	-11.5
2-Amino-4,5-dimethyl-thiophene-3-carbonitrile	616-364-4	766-36-9	766369	3722	Reach_4435	3090	125	83.2	1.5E-01	1.9E+04	1.1E+01			3.5E-06	1.1E-06	3.5E-06				16%	-10.0	-9.9	-11.7
4-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexan-1-ol	201-627-4	85-73-4	85734	3897	Reach_300	3091	403	287.4	3.2E-13	3.4E+01	3.8E+02	3.56		1.1E-06	3.5E-07	1.1E-06				18%	-9.9	-9.9	-11.5
2,3,4,6-tetrakis-O-(2,2-dimethylpropanoyl)-α-D-glucopyranosyl	686-241-8	81058-27-7	81058277	3800	Reach_4632	3092	580	193.3	1.1E-07	3.1E-03	3.2E+05			3.5E-06	3.5E-07	1.1E-06				18%	-9.9	-9.9	-11.6
citronellyl acetate	205-775-0	150-84-5	150845	2012	Reach_1206	3093	198	-7.4	7.0E+00	5.2E+01	3.6E+04			3.5E-06	3.5E-07	1.1E-06				16%	-10.1	-9.9	-11.7
608-993-8	609-521-3	38109-77-2	38109772	2817	Reach_4304	3094	140	46.9	1.3E+00	7.5E+05	7.4E-01	0	7.96	3.5E-06	3.5E-07	1.1E-06				17%	-10.1	-9.9	-11.6
trifluoro(trifluoromethoxy)ethylene	214-703-7	1187-93-5	1187935	1678	Reach_1668	3095	166	-133.2	2.1E+05	4.2E+02	2.6E+01			3.5E-07	1.1E-07	3.5E-07				22%	-10.2	-9.9	-12.7
2,4,6-triisopropyl-m-phenylene diisocyanate	251-908-0	34274-28-7	34274287	5851	Reach_2674	3096	316	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				23%	-9.8	-9.9	-11.0
dibutyl terephthalate	217-803-9	1962-75-0	1962750	525	Reach_1740	3097	278	6.0	3.4E-02	8.2E+00	4.1E+04			8.8E-07	1.1E-07	3.5E-07				17%	-10.1	-9.9	-11.5
1-(allyloxy)-2-methyl-1-oxopropan-2-yl 2-chloro-5-nitrobenzoa	221-423-9	3089-16-5	3089165	2614	Reach_1915	3098	381	253.7	6.0E-13	5.1E-03	9.3E+04			1.1E-07	1.1E-08	3.5E-08				15%	-10.1	-9.9	-11.7
pyrrolidine	204-648-7	123-75-1	123751	1774	Reach_1057	3099	71	-36.0	8.9E+03	6.3E+05	5.0E+00		3.1	1.1E-05	3.5E-07	1.1E-06				14%	-10.1	-9.9	-11.7
ethisterone	603-010-9	124750-51-2	124750512	1794	Reach_4110	3100	558	302.1	3.0E-14	1.8E-07	2.5E+08	0		3.5E-07	1.1E-08	3.5E-08				17%	-9.1	-9.9	-11.6
4-phenylbutan-2-one	219-847-4	2550-26-7	2550267	2437	Reach_1838	3101	148	12.8	8.7E+00	2.5E+02	9.1E+01			3.5E-07	1.1E-07	3.5E-07				16%	-10.1	-9.9	-11.2
N-(3-{[5-bromo-1-(2,6-dichlorobenzoyl)-1H-pyrrolo[2,3-b]pyrid	202-765-8	99-55-8	99558	1088	Reach_530	3102	152	84.5	7.8E-02	6.0E+02	1.0E+02	0	12	2.9E-09	3.5E-08	1.1E-07				22%	-9.3	-9.9	-11.0
1,3-bis(trimethylsilyl)urea	242-177-9	18297-63-7	18297637	2176	Reach_2457	3103	204	60.7	1.0E+00	4.1E+01	1.5E+02	14.3	13.9	1.1E-06	1.1E-07	3.5E-07				15%	-10.1	-9.9	-11.4
estra-4,9-diene-3,17-dione	700-798-7	877399-00-3	877399003	3941	Reach_4997	3104	380	171.7	1.7E-05	4.3E-01	1.3E+05			1.1E-06	1.1E-07	3.5E-07				16%	-10.1	-9.9	-11.7
607-173-7	607-977-8	26650-09-9	26650099	2481	Reach_4256	3105	405	18.1	8.4E+01	3.0E-01	5.9E+05	0		3.5E-07	1.1E-07	3.5E-07				14%	-9.0	-9.9	-11.8
tert-butyl [(3S)-3-amino-2-oxo-2,3,4,5-tetrahydro-1H-1-benzaz	609-723-1	39590-81-3	39590813	2842	Reach_4308	3106	102	22.2	4.1E+00	4.6E+05	1.1E+00		0	3.5E-06	3.5E-07	1.1E-06				16%	-9.2	-9.9	-11.7
L-menthan-3-one	237-926-1	14073-97-3	14073973	1929	Reach_2357	3107	154	-1.8	4.9E+01	7.4E+02	7.4E+02			1.1E-06	3.5E-07	1.1E-06				15%	-10.1	-9.9	-11.3
1,1,1,3,5,5,5-heptamethyl-3-[(trimethylsilyl)oxy]trisiloxane	241-867-7	17928-28-8	17928288	2158	Reach_2448	3108	311	-36.3	1.0E+02	2.4E-02	1.4E+08			3.5E-09	3.5E-09	3.5E-09				24%	-10.1	-9.9	-11.6
1-(2,3-dichlorophenyl)piperazine	609-736-2	39672-75-8	39672758	2847	Reach_4311	3109	415	212.7	2.5E-10	4.4E+01	2.8E+02		0	1.1E-06	1.1E-07	3.5E-07				19%	-9.8	-9.9	-11.5
benzyl methacrylate	275-639-3	71566-54-6	71566546	3584	Reach_2927	3110	926	349.8	2.2E-33	1.1E-12	2.1E+15			3.5E-07	1.1E-08	3.5E-08				15%	-10.1	-9.9	-11.3
octa-1,7-diene	218-915-0	2280-49-1	2280491	2338	Reach_1781	3111	383	185.5	1.2E-06	1.7E-01	3.3E+04			3.5E-06	1.1E-07	3.5E-07				21%	-10.2	-9.9	-12.9
609-734-1	601-431-2	1164-92-7	1164927	1649	Reach_4088	3112	332	144.6	8.6E-05	5.3E+00	1.2E+04	0		3.5E-07	3.5E-08	1.1E-07				19%	-9.6	-9.9	-11.5
trimethoxypropylsilane	213-926-7	1067-25-0	1067250	1445	Reach_1638	3113	164	-35.2	6.8E+02	5.1E+03	2.0E+00			1.1E-06	3.5E-07	1.1E-06				15%	-10.2	-9.9	-11.6
diacetoxydi-tert-butoxysilane	236-112-3	13170-23-5	13170235	1851	Reach_2324	3114	292	1.7	1.8E+00	1.1E+02	2.6E+01			1.1E-06	3.5E-07	1.1E-06				15%	-10.1	-9.9	-11.4
3,5,6-tri-O-benzyl-D-glucofuranose	601-694-3	120279-88-1	120279881	1707	Reach_4101	3115	263	174.9	1.0E-05	1.7E+02	1.9E+01	8.6		1.1E-06	3.5E-07	1.1E-06				16%	-9.1	-9.9	-11.7
2-phenylpropan-2-ol	210-539-5	617-94-7	617947	3354	Reach_1437	3116	136	8.3	6.2E+00	4.1E+04	8.9E+01	14.9		1.1E-06	1.1E-07	3.5E-07				14%	-10.1	-9.9	-11.8
ethyl 4-methyloxazole-5-carboxylate	221-341-3	3071-32-7	3071327	2610	Reach_1911	3117	138	21.1	1.7E+01	8.2E+03	5.0E+01		0	3.5E-07	3.5E-08	1.1E-07				14%	-9.0	-9.9	-11.9
methylcyclopentadiene	247-724-5	26472-00-4	26472004	2470	Reach_2582	3118	160	17.8	3.6E+01	1.4E+01	1.8E+04			1.1E-07	3.5E-08	3.5E-08				23%	-10.2	-9.9	-12.1
perhydropyrimidin-2-one	615-083-4	70223-33-5	70223335	3558	Reach_4408	3119	170	77.4	2.5E-01	1.9E+04	1.3E+01	4.74	0	1.1E-06	3.5E-07	1.1E-06				14%	-9.1	-9.9	-11.9
2-(2-piperazin-1-ylethoxy)ethanol	214-275-1	1119-34-2	1119342	5608	Reach_1653	3120	211	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				14%	-8.9	-9.9	-12.0
phenethyl acetate	606-942-4	221615-75-4	221615754	2321	Reach_4227	3121	289	175.7	6.5E-06	2.0E+02	2.0E+01			1.1E-06	3.5E-08	1.1E-07				15%	-10.2	-9.9	-11.5
nandrolone	256-841-0	50910-55-9	50910559	3023	Reach_2767	3122	279	110.7	7.2E-03	8.7E+01	3.7E+02	0		3.5E-06	3.5E-07	1.1E-06				16%	-9.2	-9.9	-11.7
triethyl phosphonoacetate	212-757-6	867-13-0	867130	3910	Reach_1572	3123	224	40.7	3.6E-01	7.6E+06	1.7E+01			3.5E-06	3.5E-07	1.1E-06				14%	-9.0	-9.9	-11.9
benzamide oxime	200-370-5	58-22-0	58220	67	Reach_46	3124	288	144.6	2.3E-06	2.4E+01	1.9E+03	16	0	3.4E-07	3.5E-08	1.1E-07				16%	-9.0	-9.9	-11.8
octanenitrile	613-941-2	66546-92-7	66546927	3476	Reach_4391	3125	183	40.1	1.2E+00	1.7E+02	2.3E+02			3.5E-06	3.5E-07	1.1E-06				16%	-10.2	-9.9	-11.7
606-947-1	606-947-1	221640-21-7	221640217	5781	Reach_4229	3126	310	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.6	-9.9	-11.6
bis(4-tert-butylphenyl)iodonium hexafluorophosphate	620-341-4	61358-25-6	61358256	5950	Reach_4565	3127	538	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.6	-9.9	-11.6

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
2,4-dihydroxy-3-methylbenzoic acid	696-298-0	144690-96-0	144690960	1980	Reach_4712	3128	432	267.5	1.2E-14	1.7E-02	2.7E+05	15.6		1.1E-06	3.5E-08	1.1E-07				14%	-9.2	-9.9	-11.9
617-590-6	700-179-1	5128-28-9	5128289	3031	Reach_4794	3129	226	171.6	1.7E-05	1.3E+02	2.8E+01	0		1.1E-06	3.5E-08	1.1E-07				16%	-9.2	-9.9	-11.7
5-nitrosalicylic acid	218-226-5	2084-69-7	2084697	2279	Reach_1757	3130	216	65.4	4.0E-01	7.0E-01	4.6E+06	0		3.5E-07	3.5E-08	1.1E-07				14%	-9.2	-9.9	-12.0
tetradecyl chloroformate	260-330-8	56677-60-2	56677602	3208	Reach_2818	3131	277	64.9	4.3E-02	1.4E-02	3.3E+06			1.1E-06	1.1E-07	3.5E-07				22%	-10.1	-9.9	-12.3
2-(dimethylamino)-2-methylpropan-1-ol	268-018-3	67989-88-2	67989882	5991	Reach_2894	3132	388	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				14%	-10.1	-9.9	-11.9
2-[2-(2-ethoxyethoxy)ethoxy]ethyl methacrylate	254-588-0	39670-09-2	39670092	2846	Reach_2727	3133	246	51.3	2.2E-01	1.2E+03	8.7E+00			3.5E-06	3.5E-07	1.1E-06				14%	-10.1	-9.9	-11.9
(E)-4-Hydroxy-3-methoxybenzaldehyde oxime	606-753-7	213967-55-6	213967556	2293	Reach_4217	3134	381	207.8	7.6E-08	9.5E-01	2.4E+01	0		1.1E-06	3.5E-08	1.1E-07				14%	-9.1	-9.9	-11.9
tetra-1-naphthyl 3,3',5,5'-tetra-tert-butyl-6,6'-dimethylbipheny	215-836-3	1424-00-6	1424006	1955	Reach_1679	3135	304	144.5	4.6E-07	4.0E+00	3.0E+03									18%	-9.6	-9.9	-11.6
8-azabicyclo[3.2.1]octan-3-ol	261-491-7	58909-56-1	58909561	3259	Reach_2833	3136	371	338.7	2.0E-15	8.7E+04	1.1E-04	2.43	7.01	3.5E-07	1.1E-07	3.5E-07				14%	-10.0	-9.9	-11.9
606-984-3	694-906-9	1363332-65-3	1363332653	5678	Reach_4684	3137	569	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				15%	-10.2	-9.9	-11.5
603-981-9	203-816-7	110-93-0	110930	291	Reach_838	3138	126	-40.0	2.4E+02	3.5E+03	1.1E+02	0		1.2E-06	3.5E-07	1.1E-06				21%	-9.5	-9.9	-11.2
1-chloro-2-(dichloromethyl)benzene	276-719-0	72576-80-8	72576808	3607	Reach_2937	3139	509	208.5	4.8E-07	1.4E-09	4.0E+15			1.1E-06	1.1E-07	3.5E-07				21%	-10.2	-9.9	-11.8
8-chloro-5,6-dihydro-11H-benzo[5,6]cyclohepta[1,2-b]pyridin-:	700-173-9	1072896-13-9	1072896139	1458	Reach_4790	3140	262	160.1	3.7E-07	1.1E+02	2.7E+02		14.6	1.1E-06	1.1E-07	3.5E-07				14%	-9.5	-9.9	-12.0
tetrahydro-2-methylfuran	202-507-4	96-47-9	96479	4147	Reach_465	3141	86	-76.2	1.4E+04	2.1E+04	2.2E+01			1.1E-06	1.1E-07	3.5E-07				15%	-10.2	-9.9	-11.9
DL-hexane-1,2-diol	230-029-6	6920-22-5	6920225	3534	Reach_2211	3142	118	1.9	2.4E+00	2.3E+04	4.9E+00	14.9		3.5E-06	1.1E-06	3.5E-06				14%	-10.1	-9.9	-11.8
2-(2,4-diaminophenoxy)ethanol dihydrochloride	266-357-1	66422-95-5	66422955	5980	Reach_2880	3143	241	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.6	-9.9	-11.6
bis(2-ethylhexyl) carbonate	238-925-9	14858-73-2	14858732	2004	Reach_2372	3144	286	12.2	3.3E+01	7.4E-01	9.1E+06			3.5E-07	3.5E-08	1.1E-07				23%	-10.1	-9.9	-12.5
octyl (R)-2-(4-chloro-2-methylphenoxy)propionate	266-358-7	66423-13-0	66423130	3473	Reach_2881	3145	327	120.6	4.8E-04	8.4E-02	4.6E+06			1.1E-06	1.1E-07	1.1E-06				21%	-9.9	-9.9	-11.3
pentaerythritol tetrakis(3-mercaptopropionate)	211-941-3	717-74-8	717748	3590	Reach_1522	3146	204	12.5	6.9E+00	6.9E-01	2.3E+06	0		3.5E-07	3.5E-08	1.1E-07				14%	-9.1	-9.9	-11.8
tetrasodium 4,4'-bis[[4-morpholino-6-(p-sulphonatoanilino)-1,:	249-323-0	28950-61-0	28950610	5821	Reach_2626	3147	1129	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.6	-9.9	-11.6
hexadecane	208-878-9	544-76-3	544763	3146	Reach_1354	3148	226	22.5	9.3E-01	5.0E-04	1.6E+08			1.1E-06	1.1E-07	3.5E-07				23%	-9.9	-9.9	-12.0
1-ethylpiperidine	242-354-0	18472-51-0	18472510	5748	Reach_2462	3149	898	0.0	0.0E+00	0.0E+00	0.0E+00		0	0.0E+00	0.0E+00	0.0E+00				15%	-10.2	-9.9	-11.3
hydrocortisone 21-acetate	200-819-5	74-88-4	74884	839	Reach_114	3150	142	-95.2	5.4E+04	1.3E+04	3.9E+01	0		4.3E-08	3.5E-09	3.5E-09				14%	-9.1	-9.9	-11.8
bis(2-ethylhexyl) 2,2'-thiobisacetate	246-131-9	24293-43-4	24293434	2384	Reach_2543	3151	375	19.8	2.0E-03	1.3E-01	5.4E+06			3.5E-07	3.5E-08	1.1E-07				22%	-10.0	-9.9	-11.2
(3-chloropropyl)diethoxymethylsilane	236-828-6	13501-76-3	13501763	1885	Reach_2339	3152	210	1.9	1.5E+01	0.0E+00	2.2E+03			1.1E-06	1.1E-07	3.5E-07				15%	-10.2	-9.9	-11.6
(Z)-3-(9-octadecenylamino)propiononitrile	200-143-0	52-51-7	52517	674	Reach_16	3153	200	90.9	8.1E-04	1.7E+05	2.3E-01		0	1.6E-08	1.1E-06	3.5E-06				22%	-10.0	-9.9	-11.4
ethyl 2-oxocyclohexanecarboxylate	695-198-4	151604-82-9	151604829	5710	Reach_4690	3154	709	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-10.2	-10.0	-11.9
N-(4-acetylaminophenyl)-3-hydroxynaphthalene-2-carboxamid	202-189-7	92-78-4	92784	4050	Reach_393	3155	298	214.0	3.9E-09	1.3E+00	1.3E+05	10.2	0	3.5E-07	3.5E-08	1.1E-07				16%	-9.4	-10.0	-11.8
696-244-6	696-244-6	84449-85-4	84449854	6052	Reach_4711	3156	666	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.6	-10.0	-11.6
2-(dibenzylamino)-1-(3,4-dihydroxyphenyl)ethanone	208-307-3	521-18-6	521186	672	Reach_1323	3157	290	146.1	1.5E-06	7.2E+00	1.2E+03	16	0	1.7E-07	1.1E-07	3.5E-07				16%	-9.4	-10.0	-11.7
N1,N5-Dibutyl-N2-(2-ethylhexanoyl)-L-glutamamide	700-210-9	1001161-63-2	1001161632	1292	Reach_4805	3158	424	170.9	2.4E-06	3.4E-02	2.6E+10	0	7.55	1.1E-06	1.1E-07	3.5E-07				16%	-9.5	-10.0	-11.8
1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene	228-846-8	6362-80-7	6362807	3414	Reach_2174	3159	236	67.0	3.0E-02	1.8E-01	3.2E+06			1.1E-06	1.1E-07	3.5E-07				21%	-10.1	-10.0	-11.5
undec-10-enal	203-973-1	112-45-8	112458	1590	Reach_908	3160	168	1.7	8.7E+00	2.1E+01	1.3E+04			3.5E-07	1.1E-07	3.5E-07				19%	-10.2	-10.0	-11.7
N-[3-(dimethoxymethylsilyl)-2-methylpropyl]ethylenediamine	257-851-8	52328-05-9	52328059	5911	Reach_2780	3161	246	0.0	0.0E+00	0.0E+00	0.0E+00		0	0.0E+00	0.0E+00	0.0E+00				14%	-10.0	-10.0	-11.9
ethyl (1R,2S)-1-amino-2-vinylcyclopropanecarboxylate sulfate (	689-958-4	1173807-85-6	1173807856	5615	Reach_4654	3162	408	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.6	-10.0	-11.6
608-209-4	608-209-4	284461-73-0	284461730	2531	Reach_4264	3163	465	269.4	5.5E-12	4.3E-01	2.0E+05	13.5	11.8	3.5E-07	3.5E-08	1.1E-07				16%	-9.6	-10.0	-11.8
2-methylquinolin-8-ol	211-448-3	645-62-5	645625	3438	Reach_1481	3164	126	-40.4	6.2E+01	1.1E+03	4.2E+02	0	0	1.1E-06	3.5E-07	1.1E-06				14%	-9.6	-10.0	-11.9
2,3-dimethylbut-1-ene	209-262-2	563-78-0	563780	3194	Reach_1374	3165	84	-116.3	3.3E+04	2.5E+02	1.3E+03			1.1E-06	3.5E-07	1.1E-06				20%	-10.3	-10.0	-13.0
2-phenyl-2-imidazoline	210-361-8	613-92-3	613923	3333	Reach_1423	3166	136	51.4	2.5E-02	3.7E+03	2.9E+00		9.4	3.5E-07	1.1E-07	3.5E-07				16%	-9.2	-10.0	-11.8
1,2-diethoxybenzene	218-089-1	2050-46-6	2050466	2269	Reach_1752	3167	166	17.0	1.1E+01	9.8E+02	4.2E+02			1.1E-06	1.1E-07	3.5E-07				15%	-10.2	-10.0	-11.5
2,5,6-trimethylcyclohex-2-en-1-one	938-119-3	1398498-88-8	1398498888	5687	Reach_5148	3168	444	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				15%	-10.2	-10.0	-11.5
3-(chloromethyl)heptane	246-273-1	24461-61-8	24461618	2394	Reach_2546	3169	165	44.6	2.0E+00	1.2E+05	3.5E+00			3.5E-06	3.5E-07	1.1E-06				22%	-10.3	-10.0	-12.8
2-isocyanatoethyl methacrylate	250-284-7	30674-80-7	30674807	2606	Reach_2648	3170	155	10.3	4.7E+01	1.1E+04	5.2E+01			3.5E-06	3.5E-07	1.1E-06				14%	-10.2	-10.0	-11.8
N-(2-hydroxyethyl)-N'-{1-methyl-1-[3-(1-methylethenyl)phenyl	200-681-6	68-22-4	68224	800	Reach_92	3171	298	161.0	3.1E-07	4.7E+00	9.8E+02	13.6	0	3.0E-07	3.5E-08	1.1E-07				14%	-9.2	-10.0	-12.0
5-phenyl-2-(2-phenylpropan-2-yl)-2H-tetrazole	611-200-8	54811-38-0	54811380	3153	Reach_4352	3172	262	102.9	9.8E-03	5.3E+01	1.8E+03			3.5E-06	3.5E-07	1.1E-06				17%	-10.2	-10.0	-11.8
icosane	800-181-3	371756-75-1	371756751	5863	Reach_5038	3173	1425	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				24%	-10.1	-10.0	-11.1
methacrylic anhydride	212-084-8	760-93-0	760930	3698	Reach_1532	3174	154	-64.9	1.2E+03	4.0E+03	1.7E+01			3.5E-06	3.5E-07	1.1E-06				14%	-10.2	-10.0	-12.0
2-methyl-3-butenenitrile	619-738-5	87305-03-1	87305031	3924	Reach_4539	3175	377	118.2	1.5E-03	9.4E+00	6.9E+02			3.5E-06	3.5E-07	1.1E-06				16%	-10.3	-10.0	-11.4
2,4,6-triisopropylaniline	209-388-8	575-61-1	575611	3232	Reach_1379	3176	222	120.9	6.0E-04	6.2E+01	5.6E+02		0	1.1E-06	1.1E-07	3.5E-07				16%	-10.2	-10.0	-11.8
615-749-4	237-196-4	13683-89-1	13683891	1902	Reach_2345	3177	167	73.7	8.0E-02	1.2E+04	8.3E+00			3.5E-06	1.1E-07	3.5E-07				14%	-10.2	-10.0	-11.9
1-(2-Ethylbutyl)cyclohexanecarbonitrile	211-014-3	627-83-8	627838	3377	Reach_1459	3178	595	211.9	1.1E-08	1.6E-10	1.3E+16			1.1E-06	1.1E-07	3.5E-07				19%	-10.2	-10.0	-11.4
progesterone	700-591-1	82203-23-4	82203234	3821	Reach_4943	3179	427	228.5	4.3E-12	3.5E+00	4.7E+02			1.1E-08	3.5E-09	1.1E-08				17%	-9.9	-10.0	-11.7
sodium nonyl sulphate	214-002-6	1072-15-7	1072157	5602	Reach_1641	3180	246	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.7	-10.0	-11.6
hexamethyldisilane	215-911-0	1450-14-2	1450142	1983	Reach_1682	3181	146	-97.8	2.8E+03	1.4E+01	1.3E+04			3.5E-09	3.5E-09	3.5E-09				24%	-10.5	-10.0	-12.7
3,3'-di-tert-butyl-5,5'-dimethoxybiphenyl-2,2'-diol	700-291-0	1000701-92-7	1000701927	5588	Reach_4845	3182	168	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				21%	-9.6	-10.0	-11.2
1,4-dimethylpiperazine	203-412-0	106-58-1	106581	1439	Reach_674	3183	114	5.4	1.3E+03	9.2E+05	4.2E-01		5.9	3.5E-06	3.5E-07	1.1E-06				14%	-10.2	-10.0	-11.9
4-chlorobenzhydryl alcohol	200-522-0	61-90-5	61905	3359	Reach_61	3184	131	262.2	7.4E-07	1.6E+04	2.6E-02	2.3		3.5E-06	3.5E-07	1.1E-06				17%	-10.1	-10.0	-11.8
2,6-difluorobenzonitrile	224-709-1	4457-71-0	4457710	2927	Reach_2039	3185	118	3.6	1.6E+00	3.4E+04	4.9E+00			1.1E-06	3.5E-07	1.1E-06				17%	-10.3	-10.0	-11.5
616-391-1	230-875-6	7347-25-3	7347253	6015	Reach_2240	3186	147	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				22%	-9.4	-10.0	-11.0
5-methylheptan-3-one	244-169-0	21049-70-7	21049707	5771	Reach_2502	3187	139	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				17%	-10.3	-10.0	-11.9
tert-butyl {(2S,3R)-3-hydroxy-4-[(2-methylpropyl)amino]-1-phe	605-203-3	160232-08-6	160232086	2072	Reach_4170	3188	336	151.8	4.9E-07	6.9E+00	1.9E+03	10.9	4.46	1.1E-06	1.1E-07	3.5E-07				15%	-9.3	-10.0	-11.9
1-methylcyclohexane-1-carboxylic acid	238-063-3	14206-62-3	14206623	5692	Reach_2359	3189	210	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-9.9	-10.0	-11.9
[[(2-ethylhexyl)oxy]methyl]oxirane	219-553-6	2461-15-6	2461156	561	Reach_1814	3190	186	4.3	2.3E+01	2.7E+00	9.3E+02			5.6E-08	1.1E-07	3.5E-07				23%	-10.3	-10.0	-12.4
3-Ethoxyestra-3,5-dien-17-one	801-163-8	571189-16-7	571189167	3225	Reach_5053	3191	308	167.0	3.4E-05	4.1E+02	1.2E+02			3.5E-07	3.5E-08	3.5E-07				17%	-10.0	-10.0	-11.8
4-vinylcyclohexene	221-209-5	3031-66-1	3031661	2591	Reach_1899	3192	114	34.4	2.3E+00	1.5E+17	7.9E-01			1.1E-06	3.5E-07	1.1E-06				20%	-10.3	-10.0	-12.9
3-[dimethyl(3-{[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulf	700-769-9	76201-56-4	76201564	3704	Reach_4989	3193	650	289.6	4.0E-17	9.5E+00	7.6E-01	-0.16		1.1E-06	1.1E-07	1.1E-06				14%	-8.9	-10.0	-12.0
methyl [(dimethoxyphosphinothioyl)thio]acetate	217-443-2	1852-17-1	1852171	2196	Reach_1727	3194	100	46.4	1.7E-02	2.7E+04	5.8E-01			3.5E-06	3.5E-07	3.5E-06				14%	-10.2	-10.0	-11.9
(3R,4S,5S,6R,7R,9R,10Z,11S,12R,13S,14R)-6-{[(2S,3R,4S,6R)-4-(	619-511-0	141573-96-8	141573968	1938	Reach_4526	3195	195	42.7	9.1E+00	2.2E+03	2.5E+00	0	0	1.1E-07	3.5E-08	3.5E-08				14%	-10.0	-10.0	-11.9
N-[3-(dimethylamino)propyl]dodecanamide	221-661-3	3179-80-4	3179804	2638	Reach_1930	3196	284	150.1	4.0E-05	8.7E-01	2.5E+04	14.8	4.8	1.1E-06	1.1E-07	3.5E-07				16%	-10.1	-10.0	-11.8
2-[(1-methylpropyl)amino]ethanol	252-471-9	35265-04-4	35265044	2726	Reach_2687	3197	117	-11.2	2.3E+01	4.3E+05	1.8E+00	15	3.9	3.5E-06	1.1E-06	3.5E-06				14%	-10.1	-10.0	-11.9
isopentylamine	203-526-0	107-85-7	107857	222	Reach_715	3198	87	-57.8	5.9E+03	2.7E+04	1.8E+01		4	2.6E-07	3.5E-07	1.1E-06				17%	-10.3	-10.0	-11.5
octyloxirane	219-295-4	2404-44-6	2404446	2370	Reach_1799	3199	156	-13.1	8.9E+01	2.3E+01	6.5E+03			1.1E-06	1.1E-07	3.5E-07				19%	-10.3	-10.0	-12.5
615-077-1	259-996-2	56107-04-1	56107041	3186	Reach_2812	3200	206	61.1	9.1E-03	3.7E+01	2.4E+04			3.5E-07	3.5E-08	1.1E-07				14%	-10.2	-10.0	-11.9
pentasodium 3,3'-({6-[(2-sulfonatoethyl)amino]-1,3,5-triazine-:	700-773-0	1342795-11-2	1342795112	5671	Reach_4990	3201	1279	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.7	-10.0	-11.7
di-tert-butyl α,α,α',α'-tetramethyl-(p-phenylenedimethylene) d	220-479-1	2781-00-2	2781002	2518	Reach_1866	3202	338	113.3	2.3E-03	5.4E-02	2.2E+07			3.5E-07	3.5E-08	1.1E-07				23%	-10.0	-10.0	-11.2

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
1-(4-chlorophenyl)sulfanyl-2-nitrobenzene	609-896-3	41202-77-1	41202771	2873	Reach_4314	3203	231	112.7	1.2E-02	1.2E+03	6.8E+02			1.1E-07	1.1E-08	3.5E-08				22%	-10.2	-10.0	-11.2
N-{3-[(5-bromo-1H-pyrrolo[2,3-b]pyridin-3-yl)carbonyl]-2,4-difl	687-535-9	122586-52-1	122586521	1754	Reach_4634	3204	737	293.0	1.3E-13	7.3E-09	1.9E+14	0	0	1.1E-06	1.1E-07	3.5E-07				16%	-9.2	-10.0	-11.9
Isononanoic acid, mixed esters with dipentaerythritol, heptano	282-775-7	84418-63-3	84418633	3863	Reach_2973	3205	328	19.9	2.2E-02	2.8E+01	8.1E+02			3.5E-06	3.5E-07	1.1E-06				14%	-10.3	-10.0	-11.9
methyl benzoylformate	203-425-1	106-70-7	106707	1444	Reach_677	3206	130	-44.6	5.5E+02	1.8E+03	2.2E+02			3.5E-06	3.5E-07	1.1E-06				14%	-10.3	-10.0	-11.9
2-methylvaleraldehyde	213-208-3	930-02-9	930029	4054	Reach_1604	3207	297	75.3	4.2E-02	1.9E-04	5.9E+08			1.1E-06	1.1E-07	3.5E-07				15%	-10.3	-10.0	-11.7
9H-carbazol-4-ol	258-034-9	52602-39-8	52602398	3064	Reach_2784	3208	183	139.6	7.4E-05	7.1E+01	5.6E+02	10		1.1E-06	3.5E-08	3.5E-07				15%	-9.4	-10.0	-11.9
methyl 4-[[(2,5-dichlorophenyl)amino]carbonyl]-2-nitrobenzoa	606-050-5	18531-99-2	18531992	2197	Reach_4190	3209	286	210.8	9.7E-10	3.8E+01	1.4E+05	9.23		1.1E-07	3.5E-09	1.1E-08				14%	-9.2	-10.0	-11.9
N-cyclohexylcyclohexanaminium (2S)-4-fluoro-4-methyl-2-({(1S	613-801-0	65473-13-4	65473134	5974	Reach_4387	3210	208	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.7	-10.0	-11.7
3-(9-anthryl)acrylaldehyde	620-448-6	566200-79-1	566200791	3207	Reach_4568	3211	568	344.5	8.5E-22	1.0E-03	3.5E+04			1.1E-07	3.5E-09	1.1E-08				17%	-10.0	-10.0	-11.8
3-nitro[1,1'-biphenyl]-4-ol	700-286-3	538-09-0	538090	3110	Reach_4841	3212	127	42.4	1.0E+00	1.7E+04	1.1E+00	15.1		3.5E-06	1.1E-06	3.5E-06				15%	-9.5	-10.0	-11.9
4,4'-Bis(methoxymethyl)biphenyl	700-008-0	3753-18-2	3753182	2802	Reach_4723	3213	242	106.5	2.1E-03	2.7E+00	2.1E+03			3.5E-07	3.5E-08	3.5E-08				17%	-10.3	-10.0	-11.8
ethyl chlorothiolformate	615-077-1	70174-49-1	70174491	3556	Reach_4407	3214	152	33.6	2.5E+00	3.7E+03	4.2E+01			3.5E-06	3.5E-07	1.1E-06				19%	-10.3	-10.0	-11.7
3,5-diiodosalicylic acid	205-124-0	133-91-5	133915	1872	Reach_1125	3215	390	163.8	1.1E-06	4.3E+01	3.8E+04	2.15		1.1E-06	3.5E-07	1.1E-06				14%	-9.4	-10.0	-11.9
N-methyl-1-(1-naphthyl)methanamine hydrochloride (1:1)	700-778-8	1064076-86-3	1064076863	5599	Reach_4991	3216	643	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.7	-10.0	-11.7
(S)-1,2-epoxypropane	201-182-6	79-16-3	79163	3767	Reach_233	3217	73	20.2	3.2E+01	2.3E+06	2.0E-01			3.5E-07	3.5E-07	1.1E-06				17%	-10.4	-10.0	-12.0
1,1'-[methylenebis(oxy)]dibutane	219-909-0	2568-90-3	2568903	2443	Reach_1840	3218	160	-20.9	1.8E+02	5.8E+02	5.6E+02			1.1E-06	1.1E-07	3.5E-07				16%	-10.3	-10.0	-11.9
decanoyl chloride	203-938-0	112-13-0	112130	1576	Reach_889	3219	191	15.9	7.1E+03	2.1E+00	2.9E+03			3.5E-07	3.5E-08	1.1E-07				22%	-10.3	-10.0	-12.8
testosterone	620-466-4	140391-39-5	140391395	1928	Reach_4573	3220	372	271.2	4.1E-12	5.6E+01	1.3E+02	13		1.1E-06	1.1E-07	3.5E-07				17%	-9.4	-10.0	-11.8
8-chloro-11-(1-methylpiperidin-4-yl)-6,11-dihydro-5H-benzo[5,	220-863-9	2921-57-5	2921575	2562	Reach_1886	3221	475	265.8	3.8E-15	2.2E+01	2.0E+02	4.22	0	3.5E-06	3.5E-07	1.1E-06				17%	-9.3	-10.0	-11.7
1,1,1-triethoxy-N,N-diethylsilanamine	700-051-5	35077-00-0	35077000	2721	Reach_4740	3222	235	32.7	4.0E+00	2.5E+02	3.2E+00		12.5	1.1E-06	3.5E-07	1.1E-06				14%	-8.9	-10.0	-12.0
1,1'-(1,1,2,2-tetramethylethylene)dibenzene	217-568-2	1889-67-4	1889674	2214	Reach_1732	3223	238	73.5	4.2E-02	6.1E-02	3.0E+06			1.1E-06	1.1E-07	3.5E-07				21%	-10.2	-10.0	-12.0
cyclopropylamine	212-142-2	765-30-0	765300	3716	Reach_1539	3224	57	-61.5	3.8E+04	1.0E+06	1.4E+00		5	3.5E-06	3.5E-07	1.1E-06				14%	-10.3	-10.0	-11.6
602-964-3	619-529-9	56914-82-0	56914820	3215	Reach_4528	3225	216	86.5	2.5E-01	8.2E+01	5.4E+01			3.5E-07	3.5E-08	1.1E-07				17%	-10.3	-10.0	-11.4
dicyclohexyl ketone	204-336-0	119-60-8	119608	353	Reach_981	3226	194	37.2	1.3E+00	2.2E+00	2.0E+04			1.0E-08	3.5E-08	1.1E-07				23%	-10.3	-10.0	-11.8
606-080-9	209-800-6	593-60-2	593602	3274	Reach_1395	3227	107	-93.5	1.4E+05	6.1E+03	3.3E+01									18%	-9.7	-10.0	-11.7
605-617-4	605-617-4	17183-98-1	17183981	2124	Reach_4180	3228	453	211.1	4.7E-08	5.8E-01	4.2E+04			3.5E-07	3.5E-08	1.1E-07				18%	-9.4	-10.0	-11.7
4-Methyl-2,6-bis[(4-methylphenyl)amino]-5-{[2-(trifluorometh	601-350-2	115241-16-2	115241162	1634	Reach_4086	3229	207	187.0	3.2E-09	5.1E+05	2.7E-03	11.9	14.9	3.5E-06	1.1E-06	3.5E-06				17%	-9.4	-10.0	-11.8
oxalyl dichloride	225-791-1	5080-22-8	5080228	3019	Reach_2076	3230	75	-42.4	3.7E+02	1.1E+05	1.4E+00			1.1E-06	3.5E-07	1.1E-06				22%	-10.5	-10.0	-12.3
614-050-1	606-524-1	203313-47-7	203313477	2260	Reach_4210	3231	333	197.4	3.7E-07	3.2E+01	3.5E+03			3.5E-07	1.1E-07	3.5E-07				21%	-9.8	-10.0	-11.4
propyltriacetoxysilane	241-816-9	17865-07-5	17865075	2155	Reach_2446	3232	248	-22.8	3.9E+00	1.6E+03	1.7E+01			3.5E-06	3.5E-07	1.1E-06				14%	-10.3	-10.1	-11.9
2,2,2-trichloro-1-phenylethyl acetate	201-972-0	90-17-5	90175	3992	Reach_360	3233	268	64.8	1.3E-01	3.0E+01	7.1E+03			1.1E-06	3.5E-07	1.1E-06				16%	-10.3	-10.1	-11.8
2-tert-butylaminoethyl methacrylate	223-228-4	3775-90-4	3775904	2806	Reach_1990	3234	185	13.1	1.7E+01	1.9E+04	1.3E+02		4.4	3.5E-06	3.5E-07	1.1E-06				14%	-10.3	-10.1	-12.0
pent-3-enenitrile	805-364-1	1170722-65-2	1170722652	5614	Reach_5064	3235	567	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				16%	-10.3	-10.1	-11.4
diethyl sulphide	206-526-9	352-93-2	352932	2728	Reach_1244	3236	90	-81.7	7.0E+03	3.5E+03	7.9E+01			1.1E-06	3.5E-07	1.1E-06				17%	-10.4	-10.1	-12.3
(2Z)-3-(3-chloro-2-fluorophenyl)-2-(4-chloro-2-fluorophenyl)ac	692-614-6	5660-53-7	5660537	3205	Reach_4677	3237	174	39.1	3.8E-01	5.6E+03	3.0E+02			1.1E-06	3.5E-07	1.1E-06				23%	-10.3	-10.1	-11.1
(vinyloxy)cyclohexane	210-484-7	616-47-7	616477	3346	Reach_1433	3238	82	2.6	6.0E+01	9.2E+04	4.1E+00			3.5E-07	3.5E-08	1.1E-07				16%	-10.4	-10.1	-12.0
dimethyl octadecylphosphonate	246-904-0	25371-54-4	25371544	2432	Reach_2567	3239	363	83.3	1.9E-04	2.0E-03	5.8E+07			1.1E-06	1.1E-07	3.5E-07				22%	-10.0	-10.1	-11.4
dimethoxymethylsilane	240-914-9	16881-77-9	16881779	2115	Reach_2429	3240	105	-100.0	1.5E+04	3.3E+04	1.1E+00			1.1E-06	3.5E-07	1.1E-06				15%	-10.4	-10.1	-12.0
614-707-2	614-707-2	68684-63-9	68684639	3524	Reach_4400	3241	300	160.1	1.3E-06	1.3E-01	1.1E+06	10		3.5E-07	3.5E-08	1.1E-07				21%	-9.7	-10.1	-11.5
ethyl 5-oxo-1-phenyl-2-pyrazoline-3-carboxylate	275-177-2	71077-34-4	71077344	6008	Reach_2926	3242	328	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				14%	-9.2	-10.1	-12.0
N-methylisopropylamine	225-266-7	4747-21-1	4747211	2967	Reach_2061	3243	73	-91.7	3.8E+04	3.5E+05	5.5E+00		2.9	3.5E-06	3.5E-07	1.1E-06				14%	-10.3	-10.1	-11.7
cineole	207-431-5	470-82-6	470826	645	Reach_1287	3244	154	8.1	2.1E+02	7.2E+00	1.3E+03			4.4E-09	3.5E-08	1.1E-07				24%	-10.4	-10.1	-12.7
p-tert-butylstyrene	217-126-9	1746-23-2	1746232	2139	Reach_1716	3245	160	0.0	3.0E+01	5.9E+00	6.3E+04			3.5E-07	3.5E-08	1.1E-07				22%	-10.4	-10.1	-12.5
1,1,3,3-tetramethylbutyl hydroperoxide	227-369-2	5809-08-5	5809085	1277	Reach_2136	3246	146	2.2	2.3E+02	2.4E+03	6.2E+02	12.7		1.1E-06	3.5E-07	1.1E-06				15%	-10.4	-10.1	-11.6
butyl hydrogen maleate	213-116-3	925-21-3	925213	4038	Reach_1596	3247	172	71.0	1.8E-01	1.6E+03	2.5E+02	3.3		3.5E-06	3.5E-07	1.1E-06				14%	-9.4	-10.1	-12.1
ethyl methyl sulphide	210-868-4	624-89-5	624895	3373	Reach_1455	3248	76	-94.5	2.0E+04	8.6E+03	2.6E+01			3.5E-07	3.5E-08	3.5E-07				19%	-10.4	-10.1	-12.3
1-[4-({4-[(E)-{5-acetamido-2-methoxy-4-[(E)-(3,6,8-trisulfo-2-n	700-803-2	14531-84-1	14531841	1984	Reach_4998	3249	272	141.9	4.2E-06	1.4E+02	4.0E+02									18%	-9.8	-10.1	-11.8
1-[4-amino-6-({4-[(E)-(4,8-disulfo-2-naphthyl)diazenyl]-8-sulfo-	215-947-7	1458-18-0	1458180	1989	Reach_1684	3250	222	116.5	8.3E-03	1.7E+03	2.3E+02									18%	-9.8	-10.1	-11.8
3,4-dichlorobut-1-ene	617-707-0	85390-93-8	85390938	3885	Reach_4471	3251	320	195.2	6.9E-10	5.4E+02	2.0E+00			1.1E-06	3.5E-07	1.1E-06				23%	-10.4	-10.1	-12.0
sodium 2-amino-5-nitrobenzenesulphonate	691-442-9	1316184-44-7	1316184447	5661	Reach_4668	3252	1047	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.8	-10.1	-11.8
2-[(o-nitrophenyl)azo]-p-cresol	615-275-8	71301-98-9	71301989	3579	Reach_4413	3253	210	86.3	1.5E-02	8.6E+02	1.1E+02	9.94		1.1E-06	1.1E-07	1.1E-06				17%	-9.6	-10.1	-11.9
1-bromobutane	203-691-9	109-65-9	109659	259	Reach_782	3254	137	-66.3	5.5E+03	6.6E+02	4.5E+02			2.3E-08	1.1E-07	3.5E-07				23%	-10.4	-10.1	-12.6
1-cyanocyclopropanaminium chloride	700-563-9	72621-59-1	72621591	3608	Reach_4936	3255	253	187.3	1.7E-06	1.3E+01	8.5E+01									18%	-9.8	-10.1	-11.7
2-Fluoro-5-(methylsulfonyl)benzoic acid	689-137-0	247569-56-8	247569568	2403	Reach_4647	3256	218	131.2	8.8E-04	1.2E+03	2.0E+00	2.66		1.1E-06	1.1E-07	3.5E-07				14%	-9.1	-10.1	-12.2
1-methyltrimethylene dimethacrylate	213-650-7	998-30-1	998301	4219	Reach_1630	3257	163	-44.7	1.1E+03	1.2E+04	1.8E+00			1.1E-06	3.5E-07	1.1E-06				14%	-10.4	-10.1	-11.9
α,α,2,6-tetrachlorotoluene	221-660-8	3179-76-8	3179768	2637	Reach_1929	3258	191	28.4	1.6E+01	1.7E+04	1.2E+01			1.1E-06	3.5E-07	1.1E-06				21%	-10.4	-10.1	-11.8
1,1,4,4-tetramethylbutane-1,4-diyl bis(2-ethylperoxyhexanoate	235-935-5	13052-09-0	13052090	1839	Reach_2322	3259	431	71.2	3.4E-04	6.1E-04	1.9E+08			1.1E-06	1.1E-07	3.5E-07				23%	-10.0	-10.1	-11.7
isopropyl acetoacetate	208-798-4	542-08-5	542085	3135	Reach_1345	3260	144	-18.7	9.6E+01	1.7E+04	1.6E+00	10.6		3.5E-06	3.5E-07	1.1E-06				14%	-10.3	-10.1	-11.9
anthracene-9-carbaldehyde	678-409-4	18402-22-7	18402227	2189	Reach_4618	3261	332	70.9	4.6E-02	1.4E+00	2.5E+08			1.1E-06	1.1E-07	3.5E-07				17%	-10.1	-10.1	-11.9
4'-hydroxyacetophenone	202-802-8	99-93-4	99934	4222	Reach_542	3262	136	51.9	2.6E-01	1.3E+04	1.5E+01	8.1		3.5E-06	3.5E-07	1.1E-06				14%	-9.9	-10.1	-12.1
(Z)-1,3-dichloropropene	233-195-8	10061-01-5	10061015	132	Reach_2279	3263	111	-72.8	3.0E+03	4.9E+03	1.9E+02			1.2E-07	1.1E-08	3.5E-08				20%	-10.4	-10.1	-12.0
benzenethiol	203-321-6	105-67-9	105679	181	Reach_647	3264	122	25.4	1.4E+01	1.7E+03	4.1E+02	10		4.5E-07	1.1E-07	3.5E-07				17%	-10.4	-10.1	-11.5
3a,4,5,6,7,7a-hexahydro-4,7-methanoinden-6-yl acetate	226-501-6	5413-60-5	5413605	3128	Reach_2106	3265	192	34.7	2.8E+00	1.1E+03	7.1E+02			3.5E-06	3.5E-07	1.1E-06				14%	-10.4	-10.1	-12.0
800-188-1	800-188-1	33626-25-4	33626254	2683	Reach_5039	3266	138	-24.5	2.9E+02	5.4E+00	2.2E+04			3.5E-07	3.5E-08	1.1E-07				22%	-10.4	-10.1	-12.9
diethyl 4,4'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[4	200-983-8	76-74-4	76744	876	Reach_176	3267	226	229.3	4.1E-08	6.8E+02	1.0E+02			3.4E-07	3.5E-07	1.1E-06				23%	-10.0	-10.1	-10.7
iodomethane	233-892-7	10416-59-8	10416598	1386	Reach_2291	3268	203	-54.8	3.2E+02	2.0E+00	5.8E+04			1.1E-06	3.5E-07	1.1E-06				23%	-10.6	-10.1	-12.7
3-methoxyestra-2,5(10)-dien-17β-ol	214-130-2	1091-93-6	1091936	1496	Reach_1645	3269	288	137.1	7.9E-06	8.0E+01	6.0E+03	16		3.5E-07	3.5E-08	1.1E-07				17%	-9.5	-10.1	-11.9
2,3,4-trichlorobut-1-ene	617-344-8	82543-09-7	82543097	3826	Reach_4452	3270	401	197.3	3.7E-09	9.2E-01	1.1E+04			1.1E-06	1.1E-07	3.5E-07				20%	-10.4	-10.1	-11.9
(ethoxymethoxy)cyclododecane	261-332-1	58567-11-6	58567116	3249	Reach_2830	3271	242	24.7	3.1E-01	2.3E+00	3.2E+05			1.1E-06	1.1E-07	3.5E-07				19%	-10.4	-10.1	-11.7
difluoroacetic acid	206-839-0	381-73-7	381737	2818	Reach_1262	3272	96	-30.9	1.2E+03	1.7E+06	7.8E-01	1.6		3.5E-06	3.5E-07	1.1E-06				14%	-9.1	-10.1	-12.1
dichlorocyclohexylmethylsilane	226-956-0	5578-42-7	5578427	3177	Reach_2125	3273	197	-20.9	1.8E+02	0.0E+00	3.2E+04			3.5E-07	1.1E-07	3.5E-07				22%	-10.4	-10.1	-12.9
608-307-7	619-021-7	94361-26-9	94361269	4104	Reach_4508	3274	223	68.6	2.5E-01	9.8E+00	2.5E+04			1.1E-06	1.1E-07	3.5E-07				15%	-10.4	-10.1	-11.6
4-tert-butyl-2-(5-tert-butyl-2-oxo-2,3-dihydro-1-benzofuran-3-	700-641-2	1261240-30-5	1261240305	1802	Reach_4957	3275	571	287.7	1.7E-14	1.3E-06	1.3E+10	8.47		1.1E-06	3.5E-08	1.1E-07				23%	-10.2	-10.1	-10.7
(2-chloro-5-iodophenyl)(4-fluorophenyl)methanone	619-596-4	915095-86-2	915095862	4017	Reach_4532	3276	361	124.7	6.0E-04	5.0E-01	1.4E+05			3.5E-08	1.1E-08	3.5E-08				22%	-10.3	-10.1	-11.3
trimethoxyoctylsilane	221-338-7	3069-40-7	3069407	2609	Reach_1910	3277	234	22.2	4.8E+00	1.0E+02	5.9E+02			1.1E-06	1.1E-07	3.5E-07				15%	-10.4	-10.1	-11.7

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
2-[(E)-(4-{[4-(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)butyl](eth	700-154-5	1034138-69-6	1034138696	1365	Reach_4782	3278	536	349.8	8.3E-18	1.4E-03	9.3E+06		11.9	3.5E-07	3.5E-08	1.1E-07				16%	-9.7	-10.2	-12.0
611-025-7	611-025-7	53651-69-7	53651697	3107	Reach_4346	3279	132	-16.0	2.1E+01	1.8E+04	2.0E+00	12.6		3.5E-06	3.5E-07	1.1E-06				14%	-10.4	-10.2	-12.1
ethyl trifluoroacetate	206-851-6	383-63-1	383631	621	Reach_1263	3280	142	-85.2	2.5E+04	7.1E+04	1.9E+01			6.8E-07	3.5E-07	1.1E-06				16%	-10.4	-10.2	-12.1
800-278-0	800-278-0	41435-93-2	41435932	2876	Reach_5040	3281	166	12.7	3.5E+01	8.1E+01	1.3E+03			1.1E-06	3.5E-07	1.1E-06				16%	-10.4	-10.2	-12.0
2-chloro-3-oxopentyl acetate	695-685-1	1360540-27-7	1360540277	5675	Reach_4693	3282	869	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				14%	-10.4	-10.2	-11.9
triethoxypropylsilane	219-842-7	2550-02-9	2550029	1250	Reach_1836	3283	206	0.1	3.3E+01	4.3E+02	6.0E+01			3.5E-07	1.1E-07	3.5E-07				17%	-10.4	-10.2	-11.7
m-bis(1-methylvinyl)benzene	223-146-9	3748-13-8	3748138	2798	Reach_1988	3284	158	-14.0	9.9E+00	5.5E+00	7.8E+04			3.5E-07	3.5E-08	1.1E-07				21%	-10.4	-10.2	-12.2
3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl methacrylate	218-407-9	2144-53-8	2144538	2294	Reach_1763	3285	432	-4.4	1.4E+02	1.5E-01	2.1E+06			3.5E-06	3.5E-07	1.1E-06				21%	-10.4	-10.2	-13.4
bisisobutyryl peroxide	222-340-0	3437-84-1	3437841	2701	Reach_1961	3286	174	-93.9	3.1E+02	2.8E+03	2.2E+02			3.5E-06	3.5E-07	1.1E-06				14%	-10.4	-10.2	-12.0
2-ethylhexyl benzoate	226-641-8	5444-75-7	5444757	3144	Reach_2113	3287	234	52.2	1.1E-01	9.0E-01	1.5E+05			1.1E-06	1.1E-07	3.5E-07				18%	-10.4	-10.2	-11.7
619-021-7	216-832-4	1678-25-7	1678257	2112	Reach_1707	3288	233	130.6	4.0E-04	2.9E+02	4.3E+02			1.1E-06	3.5E-07	1.1E-06				16%	-10.4	-10.2	-11.6
p-mentha-1,4(8)-diene	209-578-0	586-62-9	586629	731	Reach_1386	3289	136	-29.5	1.3E+02	1.8E+01	7.6E+04			5.6E-07	1.1E-07	3.5E-07				21%	-10.5	-10.2	-12.7
theophyllin-7-ylacetic acid	700-009-6	144333-84-6	144333846	1975	Reach_4724	3290	236	146.9	6.1E-04	4.4E+03	1.5E-01	0		1.1E-06	1.1E-07	3.5E-07				14%	-8.9	-10.2	-12.3
2-methoxy-5-(2-oxopropyl)benzenesulfonamide	611-489-0	57260-71-6	57260716	3227	Reach_4360	3291	186	65.1	1.1E+00	6.1E+03	1.3E+01	0		1.1E-06	3.5E-07	1.1E-06				14%	-9.2	-10.2	-12.3
methylphosphonous dichloride	700-007-5	95709-83-4	95709834	4130	Reach_4722	3292	362	224.3	7.1E-10	7.8E-01	3.7E+05			1.1E-06	3.5E-08	1.1E-07				24%	-10.6	-10.2	-12.6
Tris{4-[(4-acetylphenyl)sulfanyl]phenyl}sulfonium hexafluoroph	700-373-6	953084-13-4	953084134	6092	Reach_4878	3293	859	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.8	-10.2	-11.8
[1R-(1α,2β,4β,6α)]-2,2,7-trimethyl-3-oxatricyclo[4.1.1.02,4]oct	208-704-1	538-75-0	538750	3114	Reach_1334	3294	206	18.8	4.5E-01	7.7E-02	6.8E+06			3.5E-07	3.5E-08	1.1E-07				17%	-10.5	-10.2	-11.9
barium bis[5-chloro-4-ethyl-2-[(2-hydroxy-1-naphthyl)azo]ben	267-122-6	67801-01-8	67801018	5987	Reach_2888	3295	917	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.9	-10.2	-11.8
1-(dichloromethyl)-2-(trichloromethyl)benzene	246-928-1	25383-06-6	25383066	2433	Reach_2568	3296	122	27.1	2.3E-02	1.4E+05	5.9E-01			3.5E-07	1.1E-07	3.5E-07				19%	-10.4	-10.2	-11.6
2-ethoxy-4,6-difluoropyrimidine	230-049-5	6925-69-5	6925695	3537	Reach_2212	3297	270	196.0	4.6E-07	4.5E+00	1.6E+03			3.5E-07	1.1E-08	3.5E-08				15%	-10.4	-10.2	-11.6
3,7-dimethyloctan-1-ol	203-374-5	106-21-8	106218	1431	Reach_658	3298	158	-13.7	4.7E+00	4.6E+01	4.4E+03	15.9		1.1E-06	3.5E-07	1.1E-06				16%	-10.5	-10.2	-11.7
1,3-butylene diacetate	201-200-2	79-37-8	79378	3773	Reach_242	3299	127	-16.4	2.5E+04	1.7E+04	1.5E-02			1.1E-07	3.5E-08	3.5E-08				14%	-10.4	-10.2	-11.9
fluoroethylene	277-620-5	73833-37-1	73833371	6018	Reach_2941	3300	401	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				20%	-10.6	-10.2	-12.4
diethyl ethoxymethylenemalonate	201-725-7	87-13-8	87138	3919	Reach_307	3301	216	-41.5	4.6E+00	1.9E+03	8.9E+00			3.5E-06	3.5E-07	1.1E-06				14%	-10.4	-10.2	-12.1
(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl (2R,5R)-5-hydroxy-1	604-569-1	147126-62-3	147126623	1996	Reach_4158	3302	288	125.5	1.9E-05	2.9E+02	9.5E+01	12.2		3.5E-06	3.5E-07	1.1E-06				14%	-9.4	-10.2	-12.1
tetrasodium 4,4'-bis[[4-[(2-hydroxyethyl)amino]-6-(m-sulphona	240-400-4	16324-27-9	16324279	5731	Reach_2418	3303	1077	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.9	-10.2	-11.9
tripotassium hydrogen ethylenediaminetetraacetate	700-414-8	23328-71-4	23328714	5784	Reach_4892	3304	406	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.9	-10.2	-11.9
N,N,N-Trimethyl-3-(octadecyloxy)propan-1-ammonium chlorid	611-909-2	59875-04-6	59875046	3292	Reach_4367	3305	159	120.5	2.8E-03	7.6E+03	2.4E+00									18%	-9.9	-10.2	-11.9
ethyl 4-hydroxy-2-methyl-2H-1,2-benzothiazine-3-carboxylate	604-604-0	147770-06-7	147770067	1998	Reach_4159	3306	481	264.2	1.3E-11	2.1E-02	9.3E+06	14.3		1.1E-06	1.1E-07	3.5E-07				14%	-9.1	-10.2	-12.3
4,6-Dinitro-2,1,3-benzoxadiazole 1-oxide	207-101-0	434-22-0	434220	2913	Reach_1274	3307	274	141.0	8.4E-06	9.0E+01	6.6E+02			3.5E-07	3.5E-08	1.1E-07				14%	-9.2	-10.2	-12.3
3-p-cumenyl-2-methylpropionaldehyde	203-161-7	103-95-7	103957	1382	Reach_617	3308	190	29.1	3.0E+03	1.7E+01	8.1E+03			3.5E-07	3.5E-08	1.1E-07				22%	-10.5	-10.2	-13.0
1,4-diethylbenzene	203-265-2	105-05-5	105055	1405	Reach_635	3309	134	-17.0	1.2E+02	3.6E+01	1.2E+04			3.5E-07	3.5E-08	1.1E-07				21%	-10.5	-10.2	-12.5
3,4-dihydro-2H-pyran	201-487-4	83-56-7	83567	3849	Reach_283	3310	160	110.5	1.7E-05	3.1E+03	1.6E+02			3.5E-06	1.1E-07	3.5E-07				15%	-10.5	-10.2	-12.2
nitroethane	201-188-9	79-24-3	79243	3769	Reach_237	3311	75	-38.8	2.7E+03	3.7E+04	2.8E+00	8.8		3.5E-06	3.5E-07	1.1E-06				14%	-10.5	-10.2	-11.8
trimethoxy(2-methylpropyl)silane	250-437-8	31024-56-3	31024563	2617	Reach_2650	3312	235	47.3	1.3E+00	8.9E+03	6.0E+00			3.5E-06	1.1E-07	3.5E-07				15%	-10.5	-10.2	-12.0
triethoxysilane	214-711-0	1189-08-8	1189088	1682	Reach_1669	3313	226	-57.0	6.5E+00	8.7E+02	1.3E+03			3.5E-06	3.5E-07	1.1E-06				15%	-10.5	-10.2	-11.8
benzyl chloroformate	240-596-1	16529-56-9	16529569	2098	Reach_2423	3314	81	-59.0	1.5E+03	8.1E+03	1.3E+01			3.5E-07	1.1E-07	3.5E-07				17%	-10.5	-10.2	-12.2
diethyl N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]b	222-158-1	3373-59-9	3373599	2685	Reach_1953	3315	133	18.6	6.0E+00	3.7E+05	1.9E-02	13.3	6.9	3.5E-06	3.5E-07	1.1E-06				14%	-9.1	-10.2	-12.3
Potassium di-tert-butyl phosphate	240-387-5	16298-03-6	16298036	2087	Reach_2417	3316	153	84.9	2.1E-01	8.7E+04	1.2E+01									18%	-9.9	-10.2	-11.9
1,1'-(1,3-dioxolane-2,2-diyldimethanediyl)bis(1H-1,2,4-triazole	254-154-0	38849-09-1	38849091	2826	Reach_2719	3317	260	134.5	2.6E-04	1.5E-01	6.6E+03		0	1.1E-06	1.1E-07	3.5E-07				14%	-9.1	-10.2	-12.3
2,4-Di-tert-butyl-5-nitrophenyl methyl carbonate	695-104-1	52980-28-6	52980286	3083	Reach_4687	3318	217	128.6	1.4E-03	1.4E+02	2.4E+01			1.1E-06	1.1E-07	3.5E-07				19%	-10.3	-10.2	-11.9
bromotrimethylsilane	224-481-3	4378-61-4	4378614	2916	Reach_2030	3319	464	251.4	9.4E-11	2.3E-07	1.3E+07			3.5E-07	1.1E-08	3.5E-08				24%	-10.8	-10.2	-12.9
4-chloro-1-(dichloromethyl)benzene	296-417-2	92671-67-5	92671675	4043	Reach_2996	3320	265	118.0	2.2E-03	2.5E+02	5.5E+01			1.1E-06	1.1E-07	1.1E-06				21%	-10.5	-10.2	-12.1
tetrapropyl orthosilicate	209-790-3	593-45-3	593453	3273	Reach_1393	3321	255	31.0	1.9E-01	2.9E-04	1.5E+09			1.1E-06	1.1E-07	3.5E-07				16%	-10.5	-10.2	-12.3
diethyl dipropylmalonate	220-928-1	2941-64-2	2941642	2565	Reach_1889	3322	125	-30.8	5.4E+02	2.8E+03	3.0E+00			1.1E-07	1.1E-07	3.5E-07				15%	-10.5	-10.2	-12.0
thioacetic acid	208-063-8	507-09-5	507095	3016	Reach_1315	3323	76	-30.2	6.1E+02	1.2E+05	2.4E+00	3.4		3.5E-06	1.1E-06	3.5E-06				14%	-9.3	-10.2	-12.1
veratric acid	617-252-8	81653-77-2	81653772	3810	Reach_4449	3324	223	300.6	3.8E-08	6.6E+02	3.5E-01	1.69		3.5E-06	3.5E-07	1.1E-06				14%	-9.5	-10.2	-12.2
1-(3-tert-butyl-5-iodo-4-methoxyphenyl)pyrimidine-2,4(1H,3H)	800-476-7	1132940-53-4	1132940534	1617	Reach_5046	3325	400	238.6	6.8E-10	1.3E-01	7.9E+03	9.06		3.5E-07	1.1E-07	3.5E-07				17%	-9.6	-10.2	-11.9
691-865-9	691-865-9	17696-64-9	17696649	2149	Reach_4672	3326	151	-36.0	1.9E+02	3.1E+03	1.1E+02			1.1E-06	3.5E-07	1.1E-06				15%	-10.5	-10.2	-11.7
sodium 3-((2,3-dicyanophenyl)sulfonyl)propane-1-sulfonate	696-126-4	886592-17-2	886592172	6076	Reach_4706	3327	336	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.9	-10.2	-11.9
1,3-dichlorobut-2-ene	606-738-5	213265-81-7	213265817	2289	Reach_4215	3328	259	119.5	7.0E-03	1.9E+01	4.5E+02			1.1E-07	1.1E-08	3.5E-08				21%	-10.6	-10.2	-12.2
2,6,8-trimethylnonan-4-ol	229-554-3	6607-34-7	6607347	3461	Reach_2196	3329	236	124.5	3.6E-05	2.2E+03	1.9E+01	0		1.1E-06	1.1E-07	3.5E-07				17%	-10.5	-10.2	-11.9
nonane	225-083-2	4651-67-6	4651676	2954	Reach_2053	3330	391	214.8	1.7E-10	1.2E+01	6.9E+04			1.1E-06	1.1E-07	3.5E-07				23%	-10.6	-10.2	-13.1
N,N'-(2,5-dimethyl-1,4-phenylene)bis[4-[(5-chloro-2-methylphe	279-211-7	79665-24-0	79665240	3779	Reach_2956	3331	782	349.8	2.5E-30	2.4E-11	8.7E+14	9.13		1.1E-07	3.5E-09	1.1E-08				24%	-10.5	-10.2	-9.0
609-534-4	609-534-4	382-26-3	382263	2819	Reach_4305	3332	232	-105.5	1.3E+05	1.1E+00	2.1E+03			1.1E-06	1.1E-07	3.5E-07				20%	-10.5	-10.3	-13.2
2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-me	200-396-7	58-73-1	58731	3253	Reach_48	3333	255	94.3	7.7E-04	1.3E+03	1.3E+03	0	5.3	1.1E-06	1.1E-07	3.5E-07				16%	-9.9	-10.3	-12.1
4-{2-[2-(2-Chloro-3-{2-[1,1-dimethyl-3-(4-sulfobutyl)-1H-benzo	700-626-0	1073607-50-7	1073607507	5603	Reach_4954	3334	845	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-9.9	-10.3	-11.9
5-[[(2-aminoethyl)thio]methyl]-N,N-dimethyl-2-furfurylamine	616-285-5	76028-96-1	76028961	3694	Reach_4430	3335	330	194.5	5.7E-07	1.8E+02	1.7E+03		13.4	1.1E-06	3.5E-07	1.1E-06				14%	-9.4	-10.3	-12.3
tetrahydro-3-methylfuran	236-537-4	13423-15-9	13423159	1876	Reach_2335	3336	86	-76.2	9.9E+03	3.4E+04	2.2E+01			3.5E-07	1.1E-07	3.5E-07				17%	-10.5	-10.3	-11.9
O,O-diisobutyl hydrogen dithiophosphate	252-549-2	35410-28-7	35410287	2731	Reach_2689	3337	439	244.4	2.2E-13	5.4E+01	1.7E+00	13.4		1.1E-06	3.5E-07	1.1E-06				16%	-10.5	-10.3	-11.8
pentadecane	211-098-1	629-62-9	629629	772	Reach_1469	3338	212	12.1	2.0E+00	1.7E-03	5.1E+07			3.1E-07	1.1E-07	3.5E-07				23%	-10.3	-10.3	-12.5
5-ethyl-5-(1-methylbutyl)-2-thiobarbituric acid	700-683-1	853950-77-3	853950773	3887	Reach_4966	3339	316	0.0	0.0E+00	0.0E+00	0.0E+00	0		1.1E-06	3.5E-08	1.1E-07				17%	-9.7	-10.3	-11.9
607-988-8	610-651-8	51336-95-9	51336959	3035	Reach_4333	3340	191	30.8	7.6E+00	4.5E+02	2.1E+02			1.1E-06	3.5E-07	1.1E-06				15%	-9.6	-10.3	-12.1
8,9-Difluoro-3-methyl-6-oxo-2,3-dihydro-6H-1-oxa-3a-aza-phe	607-317-9	24085-06-1	24085061	2372	Reach_4237	3341	250	28.6	6.5E-02	2.0E+03	2.3E+01	0	0	1.1E-06	1.1E-07	3.5E-07				14%	-9.4	-10.3	-12.3
2,3-epoxybutane	276-173-3	71902-23-3	71902233	3594	Reach_2933	3342	271	182.0	3.3E-06	5.6E+01	7.8E+03			1.1E-06	1.1E-07	3.5E-07				15%	-10.5	-10.3	-11.9
6-methylhept-5-en-2-one	272-574-2	68890-66-4	68890664	5998	Reach_2911	3343	298	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				15%	-10.5	-10.3	-11.7
4'-ethoxy-3-hydroxy-2-naphthanilide	212-157-4	766-05-2	766052	873	Reach_1541	3344	109	-16.0	6.2E+01	1.2E+03	1.3E+02	0		4.1E-07	1.1E-07	3.5E-07				19%	-9.6	-10.3	-11.9
di-tert-pentyl peroxide	234-042-8	10508-09-5	10508095	1406	Reach_2293	3345	174	-19.0	3.3E+02	2.8E+01	2.7E+04			3.5E-07	1.1E-07	3.5E-07				22%	-10.6	-10.3	-12.9
ethyl (3S)-9,10-difluoro-3-methyl-7-oxo-2,3-dihydro-7H-[1,4]ox	242-500-3	18683-91-5	18683915	2204	Reach_2467	3346	378	181.5	5.4E-08	1.8E+02	1.3E+03		4.86	3.5E-06	1.1E-06	3.5E-06				14%	-9.3	-10.3	-12.3
619-072-5	224-262-2	4271-96-9	4271969	2897	Reach_2024	3347	112	15.0	4.1E+02	3.1E+04	2.2E+01	0		3.5E-06	3.5E-07	1.1E-06				14%	-9.7	-10.3	-12.4
5-bromo-1H-pyrrolo[2,3-b]pyridine	700-129-9	2004-62-8	2004628	2249	Reach_4772	3348	222	127.1	3.6E-04	5.6E+04	2.0E+00		5.63	3.5E-07	1.1E-07	3.5E-07				16%	-9.5	-10.3	-12.2
4-[[4-(aminocarbonyl)phenyl]azo]-3-hydroxy-N-(2-methoxyphe	804-749-1	1216942-02-7	1216942027	1733	Reach_5058	3349	446	278.8	1.2E-12	4.0E-03	3.2E+04	10.8	7.39	1.1E-06	1.1E-07	3.5E-07				16%	-10.0	-10.3	-12.2
N-[2-[4-(aminosulphonyl)phenyl]ethyl]-5-chloro-2-methoxyben	700-141-4	117570-53-3	117570533	1659	Reach_4778	3350	282	189.8	1.1E-06	2.1E+01	2.3E+04	3.37	14.7	3.5E-06	1.1E-07	3.5E-07				14%	-9.5	-10.3	-12.3
4-[[5-[[[4-(aminocarbonyl)phenyl]amino]carbonyl]-2-methoxyp	261-785-5	59487-23-9	59487239	3279	Reach_2837	3351	654	349.8	3.8E-25	8.6E-04	1.2E+07	9.39	13.7	3.5E-07	1.1E-08	3.5E-08				22%	-10.0	-10.3	-11.4
2-Methoxy-4-(trifluoromethyl)pyridine	619-682-1	224049-04-1	224049041	2333	Reach_4535	3352	298	186.1	2.7E-08	1.1E+01	1.7E+02		12.3	1.1E-07	1.1E-08	3.5E-08				17%	-10.6	-10.3	-12.0

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
isopentyl laurate	228-626-1	6309-51-9	6309519	3394	Reach_2164	3353	270	44.4	7.2E-02	1.3E-01	1.5E+07			1.1E-06	1.1E-07	3.5E-07				22%	-10.4	-10.3	-12.1
Benzyl {5-[N-acetyl(hydroxy)amino]pentyl}carbamate	700-416-9	92700-68-0	92700680	4044	Reach_4893	3354	294	174.1	2.9E-08	9.9E+02	5.2E+01	8.6		1.1E-06	1.1E-07	3.5E-07				14%	-9.3	-10.3	-12.2
dodecyloxirane	221-781-6	3234-28-4	3234284	2647	Reach_1935	3355	212	30.8	2.1E+00	8.5E-03	5.9E+05			3.5E-07	3.5E-08	1.1E-07				23%	-10.6	-10.3	-13.1
619-402-8	619-402-8	99189-60-3	99189603	4198	Reach_4517	3356	199	160.3	8.8E-05	1.8E+03	2.0E+01	4.73	14.5	1.1E-06	3.5E-07	1.1E-06				14%	-9.4	-10.3	-12.2
chlorocyclopentane	200-740-6	70-54-2	70542	3565	Reach_97	3357	146	299.1	6.1E-07	1.3E+05	1.0E-03			3.5E-06	3.5E-07	1.1E-06				21%	-10.6	-10.3	-12.7
2-ethylhex-2-enal	213-138-3	926-57-8	926578	4041	Reach_1597	3358	125	-69.2	1.3E+03	1.5E+03	6.9E+02			1.1E-07	1.1E-08	3.5E-08				15%	-10.5	-10.3	-11.7
2-ethylhexenal	266-097-9	66063-15-8	66063158	3459	Reach_2875	3359	210	71.1	1.3E-01	7.0E+02	9.1E+03			1.1E-07	1.1E-08	3.5E-08				15%	-10.5	-10.3	-11.7
3,3'-(hexane-1,6-diyldiimino)dipropanenitrile	700-374-1	70918-00-2	70918002	3575	Reach_4879	3360	248	153.8	7.6E-05	9.9E+02	1.1E+00		6.39	1.1E-06	1.1E-07	3.5E-07				16%	-9.4	-10.3	-12.2
tetradecyloxirane	203-783-9	110-61-2	110612	1525	Reach_820	3361	80	-0.8	8.3E-01	4.7E+04	2.3E-01			3.5E-07	1.1E-07	3.5E-07				22%	-10.5	-10.3	-13.0
5-[4'-(Bromomethyl)biphenyl-2-yl]-1-trityl-1H-tetrazole	250-185-9	30414-54-1	30414541	2596	Reach_2646	3362	144	-7.5	7.9E+01	1.3E+04	1.9E+00			1.1E-06	3.5E-07	1.1E-06				23%	-10.1	-10.3	-11.0
3-Chloro-N-hydroxy-2,2-dimethylpropanamide	805-721-1	57625-74-8	57625748	3234	Reach_5070	3363	178	17.5	8.3E+00	2.0E+02	8.9E+02	0		1.1E-06	1.1E-07	3.5E-07				16%	-9.4	-10.3	-12.2
isopropylcyclohexane	219-641-4	2489-05-6	2489056	5579	Reach_1817	3364	447	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				24%	-10.6	-10.3	-13.0
bis[2,2,6,6-tetramethyl-1-(octyloxy)piperidin-4-yl] decanedioat	700-529-3	4224-62-8	4224628	2891	Reach_4923	3365	151	55.5	1.3E+00	1.8E+03	2.0E+02			3.5E-06	3.5E-07	1.1E-06				24%	-10.5	-10.3	-10.0
Ethyl 4-oxo-1,4-dihydroquinoline-3-carboxylate	604-355-8	143418-49-9	143418499	1966	Reach_4151	3366	176	91.2	2.3E-03	0.0E+00	1.9E+02	7.6	0	1.1E-06	1.1E-07	3.5E-07				14%	-9.4	-10.3	-12.3
N-tert-butylacrylamide	203-505-6	107-58-4	107584	1466	Reach_712	3367	127	57.0	3.9E-01	6.6E+03	1.0E+01	15.1	14.4	3.5E-06	3.5E-07	1.1E-06				14%	-10.3	-10.3	-12.3
630-348-4	685-497-8	850348-10-6	850348106	6057	Reach_4631	3368	1252	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				14%	-9.7	-10.3	-12.3
1-(allyloxy)-2-methyl-1-oxopropan-2-yl 2-chloro-5-isocyanatob	695-953-8	204918-22-9	204918229	2267	Reach_4698	3369	324	58.1	9.0E-03	1.9E+01	2.1E+04			1.1E-06	1.1E-07	3.5E-07				16%	-10.5	-10.3	-12.1
(6R,7R)-7-[[(2Z)-2-(2-amino-1,3-thiazol-4-yl)-2-(methoxyimino)	616-651-4	787582-75-6	787582756	3756	Reach_4443	3370	498	194.5	3.9E-07	1.4E-04	3.5E+09	0	0	1.1E-06	3.5E-08	1.1E-07				19%	-9.5	-10.3	-11.9
octyl octanoate	218-980-5	2306-88-9	2306889	2344	Reach_1782	3371	256	53.6	1.8E-01	2.6E-01	5.8E+06			1.1E-06	1.1E-07	3.5E-07				21%	-10.5	-10.3	-12.3
1-(3-(2-methoxy-5-nitrophenoxy)propyl)-4-methylpiperazine	609-748-8	39856-50-3	39856503	2851	Reach_4312	3372	203	76.8	5.7E-01	7.6E+02	3.2E+01		0	1.1E-06	1.1E-07	3.5E-07				14%	-9.4	-10.3	-12.3
nonanal	601-329-8	114798-26-4	114798264	1626	Reach_4084	3373	423	299.9	7.3E-16	2.8E-03	1.0E+04			1.1E-07	1.1E-08	1.1E-08				18%	-10.6	-10.3	-12.1
604-275-3	611-210-2	54914-95-3	54914953	5927	Reach_4353	3374	209	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				18%	-10.6	-10.3	-12.1
α,α-dichlorotoluene	259-173-8	54464-54-9	54464549	3145	Reach_2799	3375	234	65.5	1.8E-01	4.3E+00	3.4E+05			1.1E-06	3.5E-07	1.1E-06				18%	-10.6	-10.3	-12.1
2,2-dimethyloxirane	629-664-5	79710-86-4	79710864	3780	Reach_4593	3376	100	-37.9	6.4E+02	6.8E+04	7.2E-01			1.1E-06	1.1E-07	3.5E-07				15%	-10.6	-10.3	-12.2
1-[3-(Hydroxymethyl)pyridin-2-yl]-4-methyl-2-phenylpiperazine	700-560-2	13062-58-3	13062583	1840	Reach_4934	3377	347	214.9	5.3E-10	5.6E+00	1.3E+04	8.79	8.44	3.5E-07	1.1E-07	3.5E-07				14%	-9.3	-10.3	-12.3
methyl 3-oxo-3-(thiophen-2-yl)propanoate	224-631-8	4431-83-8	4431838	2921	Reach_2034	3378	164	-9.5	1.2E+02	8.7E+04	1.8E-01	0		3.5E-07	1.1E-07	3.5E-07				14%	-10.5	-10.3	-12.4
4-hydroxy-3,5-dimethoxybenzonitrile	700-251-2	72684-95-8	72684958	3609	Reach_4822	3379	179	99.3	8.1E-03	2.7E+03	1.8E+01	8.3		1.1E-06	1.1E-07	3.5E-07				14%	-9.7	-10.3	-12.3
2-[methyl[(nonafluorobutyl)sulphonyl]amino]ethyl acrylate	266-733-5	67584-55-8	67584558	3497	Reach_2886	3380	411	85.6	9.2E-02	9.4E+00	1.5E+04			3.5E-06	3.5E-07	1.1E-06				15%	-10.6	-10.3	-12.1
barium bis[2-[(2-hydroxynaphthyl)azo]naphthalenesulphonate	214-160-6	1103-38-4	1103384	5606	Reach_1646	3381	892	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-10.0	-10.3	-12.0
(1R)-2-{[2-(4-aminophenyl)ethyl]amino}-1-phenylethanol hydr	611-111-4	54197-66-9	54197669	3132	Reach_4349	3382	163	145.0	1.1E-04	7.9E+03	1.1E+01	10.2	12.3	1.1E-05	1.1E-06	3.5E-06				14%	-9.3	-10.3	-12.3
2-[4-(Dibenzo[b,f][1,4]thiazepin-11-yl)piperazin-1-yl] ethanol	600-417-3	103312-62-5	103312625	1363	Reach_4063	3383	290	211.9	4.1E-08	3.0E+00	1.2E+04	12.2	9.58	3.5E-07	3.5E-08	1.1E-07				14%	-9.5	-10.3	-12.3
2-chloro-2-methylpropane	213-212-5	930-28-9	930289	4056	Reach_1605	3384	105	-68.5	2.7E+03	3.7E+02	7.4E+02			3.5E-07	1.1E-07	3.5E-07				22%	-10.6	-10.3	-13.1
trifluoro(trifluoromethyl)oxirane	207-050-4	428-59-1	428591	2900	Reach_1270	3385	166	-89.5	5.5E+05	7.5E+01	5.2E+01			3.5E-07	1.1E-07	3.5E-07				22%	-10.6	-10.3	-13.2
1,4-diisopropylbenzene	202-826-9	100-18-5	100185	1296	Reach_550	3386	162	-16.1	2.9E+01	1.2E+00	7.9E+04			3.5E-07	3.5E-08	1.1E-07				22%	-10.6	-10.3	-13.0
ethyl 2-methylbutyrate	231-225-4	7452-79-1	7452791	3639	Reach_2252	3387	130	-56.1	1.1E+03	3.3E+03	1.8E+02			3.5E-06	3.5E-07	1.1E-06				14%	-10.6	-10.3	-12.3
607-317-9	200-517-3	61-76-7	61767	5952	Reach_60	3388	204	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				14%	-10.4	-10.3	-12.3
1,1,1,3,3,3-hexafluoropropan-2-ol	228-705-0	6330-25-2	6330252	3398	Reach_2165	3389	98	73.3	2.4E-01	1.5E+05	3.6E-01	12.2		1.1E-06	1.1E-07	3.5E-07				22%	-10.6	-10.3	-12.7
2-chloro-N-cyclohexyl-N-(cyclohexylcarbamoyl) acetamide	202-479-3	96-12-8	96128	1045	Reach_451	3390	236	-6.9	5.9E+01	2.6E+02	4.8E+02	0	0	1.5E-08	1.1E-08	3.5E-08				14%	-9.8	-10.3	-12.3
2,3-dichloropropene	696-185-6	1407097-19-1	1407097191	5683	Reach_4137	3391	467	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				23%	-10.7	-10.3	-12.6
1-[1,6-dimethyl-3-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]eth	700-585-9	35786-94-8	35786948	2749	Reach_4941	3392	164	52.9	6.3E-01	7.2E+02	1.1E+04			1.1E-06	1.1E-07	3.5E-07				19%	-10.6	-10.3	-11.8
1-isopropyl-4-methylcyclohexane	202-790-4	99-82-1	99821	4218	Reach_539	3393	140	-52.9	2.5E+02	2.9E-01	8.3E+04			3.5E-07	3.5E-08	1.1E-07				23%	-10.6	-10.3	-13.2
3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-on	208-796-3	542-02-9	542029	3133	Reach_1343	3394	125	104.6	6.4E-02	1.9E+05	1.7E+00			1.1E-07	3.5E-08	1.1E-07				18%	-10.6	-10.3	-12.3
tetrahydro-4-methylene-2-(2-methyl-1-propenyl)-2H-pyran	700-013-8	95709-82-3	95709823	4129	Reach_4725	3395	332	218.2	1.9E-09	3.4E-01	3.5E+03			3.5E-06	3.5E-08	1.1E-07				15%	-10.6	-10.3	-11.8
N-[3-(Triethoxysilyl)propyl]formamide	607-654-1	252285-60-2	252285602	2423	Reach_4245	3396	369	244.2	2.7E-11	1.1E+00	1.9E+04	10	10.7	3.5E-07	1.1E-08	3.5E-08				14%	-9.2	-10.3	-12.3
(1E)-1-(1-Naphthyl)ethanone oxime	613-906-1	66212-25-7	66212257	3467	Reach_4390	3397	326	178.7	9.7E-08	1.0E+00	4.5E+02	13.9		1.1E-06	3.5E-07	1.1E-06				15%	-9.8	-10.3	-12.2
α-[(benzyl-tert-butylamino)methyl]-m-xylene-4,α,α'-triol	246-013-7	24085-03-8	24085038	2371	Reach_2537	3398	329	200.5	7.4E-10	1.2E+02	3.6E+02	9.97	6.81	1.1E-06	1.1E-07	3.5E-07				15%	-9.5	-10.4	-12.2
tricyclo[3.3.1.13,7]decane	266-100-3	66068-84-6	66068846	3460	Reach_2876	3399	236	87.6	1.6E-03	1.9E+01	3.2E+05			1.1E-06	1.1E-07	3.5E-07				24%	-10.6	-10.4	-12.1
1-(4-methyl-2-nitrophenylazo)-2-naphthol	219-372-2	2425-85-6	2425856	2382	Reach_1806	3400	307	200.3	3.5E-08	5.4E+00	2.8E+06	8.58		3.5E-06	3.5E-08	1.1E-07				20%	-10.2	-10.4	-12.0
cyclohexyl(ethyl)amine	226-733-8	5459-93-8	5459938	688	Reach_2115	3401	127	-23.4	2.8E+02	2.9E+02	3.9E+02		3	4.1E-07	3.5E-07	1.1E-06				18%	-10.6	-10.4	-12.3
N,N'-hexane-1,6-diylbis[2,2-dimethyl-3-(morpholin-4-yl)propan	700-570-7	1217271-49-2	1217271492	1736	Reach_4938	3402	423	187.7	5.5E-07	1.7E+00	8.9E+02		6.18	1.1E-06	1.1E-07	3.5E-07				15%	-9.7	-10.4	-12.3
triammonium hydrogen ethylenediaminetetraacetate	240-073-8	15934-01-7	15934017	5727	Reach_2405	3403	343	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-10.0	-10.4	-12.0
4-(4-Nitrophenyl)morpholin-3-one	610-199-1	446292-04-2	446292042	2928	Reach_4325	3404	222	150.1	1.5E-04	4.7E+03	5.6E+00			1.1E-06	1.1E-07	3.5E-07				14%	-9.4	-10.4	-12.4
2,2-difluoro-benzo[1,3]dioxole-4-carbaldehyde	700-476-6	119895-68-0	119895680	1701	Reach_4908	3405	186	52.2	2.4E+00	8.3E+02	2.2E+03			1.1E-06	3.5E-07	1.1E-06				15%	-10.6	-10.4	-12.1
4-chloro-2,3-dimethylpyridine 1-oxide	700-045-2	104966-97-4	104966974	1404	Reach_4737	3406	338	195.0	5.6E-09	6.1E+00	2.3E+04		0	1.1E-06	3.5E-07	1.1E-06				16%	-10.6	-10.4	-12.2
5-aminonaphthalene-2-sulphonic acid	204-351-2	119-79-9	119799	1699	Reach_986	3407	223	173.4	7.0E-08	2.3E+03	1.2E-01	0.32	10.3	1.1E-06	1.1E-07	3.5E-07				14%	-9.2	-10.4	-12.5
N-(4-bromobenzyl)-N-pentanoyl-L-valine	601-254-0	113479-65-5	113479655	1621	Reach_4081	3408	171	290.4	2.6E-06	1.1E+02	7.6E-03	1.88		3.5E-06	3.5E-07	1.1E-06				14%	-9.8	-10.4	-12.3
allyl hexanoate	223-242-0	3779-63-3	3779633	2809	Reach_1991	3409	505	307.3	1.3E-14	2.8E-03	6.5E+09			1.1E-06	1.1E-07	3.5E-07				15%	-10.7	-10.4	-12.2
dicyclohexylcarbodiimide	243-411-2	19894-99-6	19894996	2245	Reach_2486	3410	152	17.8	1.4E+02	5.5E+02	7.4E+02			3.5E-07	1.1E-07	3.5E-07				23%	-10.6	-10.4	-12.7
2-phenylethyl cyanoacetate	643-078-7	87855-59-2	87855592	3943	Reach_4612	3411	242	107.6	4.7E-03	0.0E+00	2.8E+00			3.5E-06	3.5E-07	3.5E-06				14%	-10.4	-10.4	-12.3
2-phenoxyaniline	620-225-3	5958-24-7	5958247	3280	Reach_4562	3412	305	203.5	1.5E-07	1.6E-01	6.9E+03		0	1.1E-07	1.1E-08	3.5E-08				14%	-9.8	-10.4	-12.4
3-cyclohexyl-2-(cyclohexylimino)-1,3-oxazolidin-4-one	700-085-0	329216-67-3	329216673	2670	Reach_4755	3413	339	206.9	6.9E-10	4.8E+03	1.7E+02		8.23	1.1E-06	1.1E-07	3.5E-07				14%	-9.8	-10.4	-12.3
N,N-dimethylbutylamine	213-156-1	927-62-8	927628	1014	Reach_1600	3414	101	-70.6	6.2E+03	2.9E+04	3.2E+01		4	6.2E-07	3.5E-07	1.1E-06				16%	-10.7	-10.4	-12.0
6-amino-4-hydroxynaphthalene-2-sulphonic acid	700-266-4	26184-62-3	26184623	2457	Reach_4830	3415	88	-63.7	9.7E+02	3.6E+04	1.8E+01	16	0	1.1E-06	3.5E-07	1.1E-06				14%	-9.3	-10.4	-12.5
[methoxy(dimethyl)silyl]methyl acetate	299-966-6	93918-85-5	93918855	4091	Reach_3003	3416	270	89.2	2.3E-03	2.9E-02	1.8E+06			1.1E-06	1.1E-07	3.5E-07				14%	-10.6	-10.4	-12.0
1,1,1,2,3-Pentachlorpropane	700-848-8	1247119-33-0	1247119330	5640	Reach_5011	3417	446	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				22%	-10.7	-10.4	-12.6
4-amino-2-(trifluoromethyl)benzonitrile	700-293-1	654-70-6	654706	3454	Reach_4847	3418	186	64.2	7.1E-01	1.1E+03	1.4E+02		13.5	1.1E-06	3.5E-07	1.1E-06				15%	-10.6	-10.4	-12.2
Methyl (3aR,7aR)-4-oxooctahydro-1H-indole-1-carboxylate	700-703-9	18667-19-1	18667191	2202	Reach_4973	3419	301	198.5	3.1E-07	4.4E+00	6.2E+04		15	1.1E-06	1.1E-07	3.5E-07				14%	-9.4	-10.4	-12.3
3,5-bis{1-[4-(propan-2-yl)phenyl]propan-2-yl}dihydro-1H-[1,3](	700-207-2	1001164-15-3	1001164153	1293	Reach_4804	3420	436	198.2	1.3E-07	6.2E-03	7.8E+08		7.89	1.1E-06	1.1E-07	3.5E-07				22%	-10.2	-10.4	-11.3
606-682-1	611-928-6	6001-74-7	6001747	5944	Reach_4369	3421	198	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				15%	-9.7	-10.4	-12.3
2,2,5,5-tetramethyl-1,4,2,5-dioxadisilinane	700-669-5	2788-28-5	2788285	5814	Reach_4964	3422	179	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				24%	-10.8	-10.4	-12.7
620-465-9	700-259-6	64464-07-9	64464079	5968	Reach_4828	3423	204	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				14%	-9.5	-10.4	-12.3
3,5,5-trimethylcyclohex-3-en-1-one	695-943-3	151006-11-0	151006110	5709	Reach_4697	3424	442	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				15%	-10.7	-10.4	-11.9
barium bis[6-chloro-4-[(2-hydroxy-1-naphthyl)azo]toluene-3-su	277-553-1	73612-34-7	73612347	6017	Reach_2940	3425	889	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-10.1	-10.4	-12.1
diisobutyl maleate	238-102-4	14234-82-3	14234823	1954	Reach_2360	3426	228	-49.2	4.5E+00	5.8E+01	1.0E+04			3.5E-06	3.5E-07	1.1E-06				15%	-10.7	-10.4	-12.1
613-906-1	700-765-7	100485-51-6	100485516	1307	Reach_4987	3427	185	78.2	2.8E-04	8.5E+01	3.9E+03	11.1		1.1E-06	3.5E-08	1.1E-07				15%	-9.7	-10.4	-12.3

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
1-({[(2,5-dioxopyrrolidin-1-yl)oxy]carbonyl}oxy)ethyl 2-methylp	700-402-2	860035-10-5	860035105	3900	Reach_4888	3428	273	168.7	3.4E-06	1.9E+04	3.9E-02			3.5E-06	3.5E-07	1.1E-06				14%	-9.3	-10.4	-12.6
3,5-Di(undecan-2-yl)dihydro-1H-[1,3]oxazolo[3,4-c][1,3]oxazol	202-657-0	98-32-8	98328	4182	Reach_504	3429	188	155.1	4.4E-05	2.0E+04	9.3E-02		11	3.5E-06	1.1E-07	3.5E-07				23%	-10.5	-10.4	-10.9
3-ethoxypregna-3,5-diene-21,17α-carbolactone	700-664-8	486455-65-6	486455656	2973	Reach_4963	3430	384	269.0	5.9E-12	4.5E-01	4.7E+03			3.5E-07	3.5E-08	1.1E-07				19%	-10.0	-10.4	-12.0
2-methyl-2,3,4,5,6,7,8,9,10,11,12,13-dodecahydro-1H-cycloper	606-858-8	21890-09-5	21890095	2310	Reach_4220	3431	220	46.0	3.3E-01	1.2E-02	1.3E+07			1.1E-06	1.1E-07	3.5E-07				22%	-10.5	-10.4	-13.0
Diethyl pyridine-2,4-dicarboxylate	680-341-5	41438-38-4	41438384	2877	Reach_4625	3432	223	18.1	4.6E-01	1.5E+03	1.4E+01		14.5	1.1E-06	1.1E-07	3.5E-07				14%	-10.6	-10.4	-12.4
chlorocyclohexane	203-113-5	103-45-7	103457	1367	Reach_606	3433	164	10.6	9.1E+00	1.3E+03	3.7E+02			1.1E-06	1.1E-07	3.5E-07				23%	-10.7	-10.4	-12.4
butyl(ethyl)amine	236-415-0	13360-63-9	13360639	1869	Reach_2330	3434	101	-54.3	3.6E+03	7.5E+04	6.2E+01		3.1	3.5E-06	3.5E-07	3.5E-07				14%	-10.6	-10.4	-12.0
[(1R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methanesulfon	700-248-6	2766-74-7	2766747	2515	Reach_4820	3435	217	96.6	3.7E-02	4.7E+02	2.6E+03									18%	-10.1	-10.4	-12.1
tert-butyl {(1S)-2-[(1S,3S,5S)-3-cyano-2-azabicyclo[3.1.0]hex-2-	687-691-8	709031-43-6	709031436	3573	Reach_4636	3436	416	224.7	2.9E-11	4.9E+01	3.4E+02	8.72		3.5E-07	3.5E-08	1.1E-07				16%	-9.5	-10.4	-12.2
N,N-dibutylbutan-1-aminium bis[2-(hydroxy-kO)benzoato(2-)-k	700-536-1	25628-08-4	25628084	5798	Reach_4926	3437	430	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-10.1	-10.4	-12.1
N,N,N-triethylethanaminium 1,1,2,2,3,3,4,4,4-nonafluorobutan	226-887-6	5534-13-4	5534134	3167	Reach_2122	3438	449	229.2	3.7E-12	1.1E+01	8.9E+02									18%	-10.1	-10.4	-12.1
2-acetamido-5-chlorobenzenesulfonic acid - pyridine (1:1)	250-882-8	31981-44-9	31981449	2641	Reach_2659	3439	358	178.1	4.2E-06	6.2E+01	1.7E+03									18%	-10.1	-10.4	-12.1
603-087-9	603-087-9	125700-67-6	125700676	6112	Reach_4111	3440	321	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-10.1	-10.4	-12.1
2,2-dimethoxy-N-{2-oxo-2-[(2-phenylethyl)amino]ethyl}ethana	700-631-8	102601-34-3	102601343	5592	Reach_4956	3441	259	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-10.1	-10.4	-12.1
690-742-7	700-789-8	14352-61-5	14352615	1967	Reach_4995	3442	156	-14.6	4.9E+01	2.6E+02	1.3E+03									18%	-10.1	-10.4	-12.1
sodium 3-(cyclohexylamino)-2-hydroxypropane-1-sulfonate	696-235-7	63432-37-1	63432371	3401	Reach_4710	3443	210	128.4	1.9E-03	3.5E+02	4.3E+02									18%	-10.1	-10.4	-12.1
L-tryptophan	254-179-7	38888-98-1	38888981	2828	Reach_2720	3444	182	29.7	1.1E+00	6.3E+00	1.4E+04	0	0	1.1E-06	1.1E-07	3.5E-07				14%	-9.1	-10.4	-12.4
Lithium naphthalene-2-carboxylate	700-252-8	53595-66-7	53595667	3106	Reach_4823	3445	198	116.9	9.7E-03	5.3E+03	6.8E+00									18%	-10.1	-10.4	-12.1
6-BROMO-4-PHENYLCHROMAN-2-ONE	610-915-2	52937-90-3	52937903	3082	Reach_4339	3446	157	4.3	2.6E+01	3.1E+03	1.3E+01			3.5E-06	3.5E-07	1.1E-06				15%	-10.3	-10.4	-12.4
estrone	200-164-5	53-16-7	53167	61	Reach_19	3447	270	153.1	6.8E-01	8.3E+00	2.7E+03	9.92		1.1E-07	1.1E-07	3.5E-07				20%	-10.7	-10.4	-12.0
5-Bromo-3-[(1R)-1-(2,6-dichloro-3-fluorophenyl)ethoxy]pyridin	689-734-6	39903-01-0	39903010	2852	Reach_4653	3448	189	102.7	2.2E-02	7.7E+03	8.7E+00		9.88	3.5E-07	3.5E-08	1.1E-07				14%	-9.9	-10.4	-12.4
4-amino-N-(2-methylquinolin-8-yl)benzenesulfonamide	604-269-0	14205-46-0	14205460	1945	Reach_4146	3449	143	-7.1	7.0E+01	7.7E+03	4.3E+00	0	5.24	3.5E-06	3.5E-07	1.1E-06				14%	-9.8	-10.4	-12.3
(2Z)-(5-amino-1,2,4-thiadiazol-3-yl){[(1-tert-butoxy-2-methyl-1-	609-518-7	38089-93-9	38089939	2815	Reach_4303	3450	343	188.3	1.8E-08	2.6E+00	1.3E+04	12.1	4.43	3.5E-07	3.5E-08	1.1E-07				14%	-9.8	-10.4	-12.3
methyl benzilate	700-294-7	109010-60-8	109010608	1492	Reach_4848	3451	290	173.7	8.5E-06	3.0E+01	4.1E+01	0		3.5E-07	1.1E-07	3.5E-07				15%	-9.7	-10.4	-12.4
3-(dodecylthio)butyronitrile	604-275-3	14214-31-4	14214314	1947	Reach_4147	3452	134	-23.8	2.9E+02	7.3E+02	4.4E+02			3.5E-07	3.5E-08	1.1E-07				20%	-10.6	-10.4	-11.9
618-972-5	618-972-5	93771-36-9	93771369	4082	Reach_4505	3453	370	191.8	1.0E-08	3.2E+00	1.5E+04	14.1		1.1E-06	1.1E-07	3.5E-07				16%	-9.6	-10.4	-12.2
680-297-7	806-599-2	33125-90-5	33125905	2675	Reach_5077	3454	407	194.3	5.9E-07	3.2E+00	7.1E+03	0	0	3.5E-07	3.5E-08	1.1E-07				16%	-9.4	-10.4	-12.3
2-(2-aminopropan-2-yl)-4-[(4-fluorobenzyl)carbamoyl]-1-meth	608-783-6	327-78-6	327786	2663	Reach_4283	3455	222	9.5	5.4E+01	6.1E+01	1.6E+04	0	0	1.1E-06	1.1E-07	3.5E-07				15%	-9.5	-10.4	-12.3
6-Iodo indazole	620-465-9	2657-85-4	2657854	2479	Reach_4572	3456	227	195.6	4.8E-07	2.0E+02	7.4E+00		9.94	1.1E-06	3.5E-07	1.1E-06				15%	-10.4	-10.4	-12.4
604-355-8	700-139-3	867022-57-9	867022579	3909	Reach_4776	3457	370	192.7	7.4E-07	2.9E+00	3.9E+04	3.2		1.1E-06	1.1E-07	3.5E-07				15%	-9.7	-10.4	-12.4
6-methyl-4-oxo-5,6-dihydro-4H-thieno[2,3-b]thiopyran-2-sulfo	700-296-8	61337-89-1	61337891	3332	Reach_4849	3458	283	175.9	1.6E-07	2.7E+04	4.3E+01	15.8		1.1E-06	1.1E-07	3.5E-07				14%	-9.7	-10.4	-12.4
propane-2-thiol	200-861-4	75-33-2	75332	3667	Reach_139	3459	76	-101.0	3.5E+04	9.0E+03	4.8E+01	10.7		1.1E-06	3.5E-07	1.1E-06				17%	-10.7	-10.4	-12.8
pentafluoroiodoethane	212-058-6	757-86-8	757868	3688	Reach_1528	3460	230	-21.0	7.2E-01	1.2E+03	2.2E+01			3.5E-06	3.5E-07	1.1E-06				23%	-10.8	-10.4	-13.1
N-[(3R,4R)-1-benzyl-4-methylpiperidin-3-yl]-2-chloro-N-methyl-	220-513-5	2787-02-2	2787022	1256	Reach_1869	3461	340	199.0	9.7E-10	3.8E+03	1.7E+03		0	3.5E-07	3.5E-08	1.1E-07				15%	-9.6	-10.4	-12.3
601-350-2	700-100-0	39716-58-0	39716580	2848	Reach_4762	3462	119	-43.8	1.7E+03	4.3E+03	7.2E+00	0	0	3.5E-06	3.5E-07	1.1E-06				14%	-9.2	-10.4	-12.4
dibenzo(b,f)cycloheptan-1-one	614-818-6	689293-69-4	689293694	3531	Reach_4401	3463	541	303.1	2.5E-14	1.2E-02	1.3E+05			3.5E-07	3.5E-08	1.1E-07				18%	-10.7	-10.4	-11.9
3-(1-pyrrolidinyl)propiophenone hydrochloride	212-633-1	833-86-3	833863	6047	Reach_1561	3464	240	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-10.1	-10.4	-12.1
4-(decanoyloxy)benzoic acid	617-941-3	86960-46-5	86960465	3914	Reach_4481	3465	292	151.1	3.1E-05	1.2E+00	2.5E+05	4.2		1.1E-06	1.1E-07	3.5E-07				15%	-9.9	-10.4	-12.4
3-phenylbutyraldehyde	240-362-9	16251-77-7	16251777	2085	Reach_2415	3466	148	1.2	1.1E+01	2.4E+03	2.8E+02			3.5E-07	1.1E-07	3.5E-07				16%	-10.7	-10.4	-11.9
N-(5-chloro-2-methoxyphenyl)-3-hydroxy-4-[[2-methoxy-5-[(pl	224-794-5	4498-67-3	4498673	2935	Reach_2041	3467	164	136.2	2.0E-03	2.8E+04	2.4E+00	2.6	7.03	3.5E-06	3.5E-07	1.1E-06				16%	-10.1	-10.4	-12.3
tert-butyl piperazine-1-carboxylate	618-533-8	90356-78-8	90356788	3999	Reach_4497	3468	398	220.4	6.2E-11	1.0E+00	2.1E+04		0	1.1E-06	3.5E-08	1.1E-07				14%	-10.7	-10.4	-12.4
dichloromethyl(3,3,3-trifluoropropyl)silane	211-623-4	675-62-7	675627	3496	Reach_1495	3469	211	-59.0	4.5E+03	0.0E+00	2.9E+03			3.5E-08	1.1E-08	1.1E-08				23%	-10.9	-10.4	-13.1
4-[2-(benzylamino)propyl]phenol	225-511-8	4890-85-1	4890851	2979	Reach_2066	3470	226	132.4	3.5E-04	2.2E+01	1.9E+04	3.58	0	1.1E-06	3.5E-07	1.1E-06				15%	-9.7	-10.4	-12.3
615-027-9	615-027-9	69904-10-5	69904105	3552	Reach_4406	3471	207	208.3	7.2E-08	3.9E+04	3.0E-01	10.1	8.59	1.1E-06	1.1E-07	3.5E-07				14%	-9.2	-10.4	-12.5
4'-chloro-3-hydroxy-2-naphthanilide	204-248-2	118-41-2	118412	1668	Reach_962	3472	212	118.7	9.2E-04	2.6E+03	2.5E+01	4.3		1.1E-06	1.1E-07	3.5E-07				19%	-9.8	-10.4	-12.0
3-chlorophthalic anhydride	620-285-0	902146-43-4	902146434	3994	Reach_4563	3473	240	129.5	1.3E-03	2.2E+03	3.8E+01			3.5E-07	3.5E-08	1.1E-07				15%	-10.7	-10.4	-12.1
608-291-1	211-814-2	698-29-3	698293	3550	Reach_1513	3474	134	98.9	8.0E-02	4.6E+04	4.7E-01			3.5E-07	1.1E-07	3.5E-07				20%	-10.7	-10.4	-12.6
1,1'-(1,3-Phenylenedicarbonyl)diazepan-2-one	700-226-6	488097-90-1	488097901	2976	Reach_4811	3475	243	83.3	2.3E-02	3.7E+04	2.6E+02		0	3.5E-06	3.5E-07	1.1E-06				15%	-9.6	-10.4	-12.3
ethyl 1-(4-methoxyphenyl)-7-oxo-6-[4-(2-oxopiperidin-1-yl)phe	253-292-9	36968-27-1	36968271	2786	Reach_2708	3476	440	321.7	5.0E-17	3.8E-01	3.5E+05		14.9	3.5E-07	1.1E-08	3.5E-08				16%	-10.0	-10.4	-12.3
oleoyl chloride	616-210-6	75302-98-6	75302986	3665	Reach_4427	3477	472	230.0	2.6E-09	6.4E-02	6.0E+05			1.1E-06	1.1E-07	3.5E-07				22%	-10.6	-10.4	-12.7
2,6,6-trimethylbicyclo[3.1.1]heptane-3-carbaldehyde	619-372-6	98730-04-2	98730042	4191	Reach_4515	3478	260	118.0	1.6E-03	2.1E+02	2.4E+02			3.5E-07	1.1E-07	3.5E-07				15%	-10.7	-10.4	-11.9
610-150-4	700-627-6	17270-01-8	17270018	2130	Reach_4955	3479	651	90.3	2.7E-06	6.8E-06	1.5E+09									18%	-10.1	-10.4	-12.1
639-259-5	639-259-5	104366-82-7	104366827	1391	Reach_4603	3480	210	136.6	1.0E-05	2.6E+03	6.3E-01	3.73	3.8	3.5E-06	3.5E-07	1.1E-06				14%	-9.3	-10.4	-12.5
N-(dimethylvinylsilyl)-1,1-dimethyl-1-vinylsilylamine	231-701-1	7691-02-3	7691023	1290	Reach_2269	3481	185	-36.2	5.3E+02	0.0E+00	2.1E+03		4.7	1.1E-06	1.1E-07	3.5E-07				19%	-10.7	-10.4	-13.1
Nonylphenol, ethoxylated	500-024-6	9016-45-9	9016459	1001	Reach_4050	3482	441	209.5	1.3E-10	1.9E-01	3.0E+04	14.9		2.5E-07	3.5E-07	1.1E-06				18%	-9.7	-10.5	-12.0
N-ethylmethacrylamine	242-217-5	18328-90-0	18328900	2182	Reach_2459	3483	99	-64.5	3.4E+03	7.1E+04	5.1E+01		3.8	1.1E-05	3.5E-07	1.1E-06				14%	-10.7	-10.5	-12.2
4,4'-methylenebis(N-sec-butylcyclohexanamine)	217-101-2	1739-84-0	1739840	2135	Reach_1715	3484	96	20.3	3.6E+01	3.7E+04	1.4E+01		5.8	3.5E-07	3.5E-08	1.1E-07				21%	-10.6	-10.5	-12.3
tert-butyl peroxyisobutyrate	239-032-7	14960-06-6	14960066	5705	Reach_2374	3485	351	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				16%	-10.7	-10.5	-12.4
Diethyl N-[4-(4-oxobutyl)benzoyl]-L-glutamate	608-229-3	2863-88-9	2863889	2540	Reach_4266	3486	300	141.1	4.1E-04	3.4E+01	4.3E+03	0		3.5E-07	3.5E-08	1.1E-07				15%	-9.7	-10.5	-12.4
betahistine	609-695-0	394735-17-2	394735172	2840	Reach_4307	3487	171	33.4	6.3E+00	7.8E+04	3.9E+01		6.3	3.5E-06	3.5E-07	1.1E-06				16%	-10.7	-10.5	-11.9
600-553-3	222-111-5	3351-05-1	3351051	1183	Reach_1952	3488	682	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				19%	-9.8	-10.5	-12.0
isovaleryl chloride	218-485-4	2162-73-4	2162734	2299	Reach_1766	3489	286	82.9	1.9E-02	6.4E-01	3.6E+07			3.5E-07	3.5E-08	1.1E-07				16%	-10.8	-10.5	-12.6
fluocortolone	806-511-2	35877-42-0	35877420	2753	Reach_5074	3490	264	141.4	9.6E-05	2.7E+02	1.6E+04	0		1.1E-06	1.1E-07	3.5E-07				14%	-9.6	-10.5	-12.3
618-883-1	617-590-6	846023-24-3	846023243	3869	Reach_4469	3491	259	177.6	7.0E-06	1.5E+03	1.4E+02			3.5E-07	1.1E-07	3.5E-07				15%	-10.5	-10.5	-12.4
606-376-8	609-972-6	41965-95-1	41965951	5883	Reach_4318	3492	208	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				15%	-9.6	-10.5	-12.3
3-benzylidenephthalide	610-717-6	5173-46-6	5173466	3045	Reach_4334	3493	270	145.4	3.1E-04	4.7E+00	2.2E+02			3.5E-07	3.5E-08	1.1E-07				15%	-10.3	-10.5	-12.4
613-901-4	613-901-4	6615-00-5	6615005	3465	Reach_4389	3494	288	163.9	2.9E-07	6.3E+01	5.9E+00	15.6		1.1E-06	1.1E-07	3.5E-07				14%	-9.5	-10.5	-12.5
o-phenethylbenzoic acid	218-121-4	2051-49-2	2051492	2270	Reach_1753	3495	214	1.7	1.1E+01	8.8E+00	2.2E+03	0		3.5E-07	3.5E-08	1.1E-07				14%	-9.9	-10.5	-12.4
5-bromo-2-nitropyridine	210-088-4	605-50-5	605505	3311	Reach_1413	3496	306	0.7	6.4E-06	1.2E+00	2.8E+05			1.1E-06	1.1E-07	3.5E-07				14%	-10.7	-10.5	-12.4
5'-chloro-3-hydroxy-2',4'-dimethoxy-2-naphthanilide	202-182-9	92-72-8	92728	4047	Reach_390	3497	358	236.1	1.0E-10	1.0E-01	5.2E+04	10.2		1.1E-06	3.5E-08	1.1E-07				17%	-9.7	-10.5	-12.2
2-chloro-3-(hydroxymethylene)cyclohex-1-ene-1-carbaldehyde	615-113-6	704-10-9	704109	3562	Reach_4409	3498	207	47.3	2.6E+00	8.2E+01	1.4E+03			1.1E-07	3.5E-08	1.1E-07				14%	-9.9	-10.5	-12.4
N-[3-({[2,2-dimethyl-3-(morpholin-4-yl)propylidene]amino}met	700-584-3	1217271-02-7	1217271027	1735	Reach_4940	3499	477	211.4	4.4E-08	2.1E-01	5.1E+05		6.18	1.1E-06	1.1E-07	3.5E-07				19%	-9.9	-10.5	-12.0
4-[(4-chloropyrimidin-2-yl)amino]benzonitrile	607-384-4	244768-32-9	244768329	2396	Reach_4240	3500	231	143.1	4.0E-04	1.3E+02	6.9E+02		11.2	3.5E-07	3.5E-08	1.1E-07				16%	-9.9	-10.5	-12.4
3-(vinyloxy)propan-1-amine	700-340-6	76524-94-2	76524942	3715	Reach_4868	3501	249	127.2	1.5E-03	1.8E+04	6.5E-01		14.5	1.1E-06	3.5E-07	1.1E-06				14%	-10.7	-10.5	-12.3
benzidine-2,2'-disulphonic acid	204-179-8	117-21-5	117215	1657	Reach_958	3502	183	50.8	4.4E-01	8.5E+01	5.1E+02	0	0	1.1E-06	1.1E-07	3.5E-07				14%	-9.2	-10.5	-12.5

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
620-466-4	284-362-7	84852-49-3	84852493	6055	Reach_2981	3503	612	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-9.5	-10.5	-12.4
3-aminopyrazine-2-carboxylic acid	226-558-7	5424-01-1	5424011	1275	Reach_2111	3504	139	118.6	1.0E-02	1.7E+05	1.5E+00	1.83	9.39	3.5E-07	3.5E-08	1.1E-07				16%	-9.5	-10.5	-12.4
617-350-0	617-350-0	82543-18-8	82543188	3831	Reach_4457	3505	391	213.0	2.4E-11	3.2E+02	8.3E+02	15.1		1.1E-06	1.1E-07	3.5E-07				15%	-9.7	-10.5	-12.3
mesterolone	253-258-3	36894-69-6	36894696	2785	Reach_2707	3506	328	228.5	4.4E-11	2.3E+01	2.6E+02	7.47		1.1E-06	1.1E-07	3.5E-07				17%	-9.8	-10.5	-12.3
methyl phenylacetate	601-621-5	119532-26-2	119532262	5623	Reach_4096	3507	268	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				14%	-10.7	-10.5	-12.3
methyl ({[(1Z)-1-(2-amino-1,3-thiazol-4-yl)-2-(1,3-benzothiazol-	204-344-4	119-70-0	119700	1698	Reach_985	3508	279	218.1	9.5E-11	2.2E+03	1.6E-03		7.26	1.1E-06	1.1E-07	1.1E-06				14%	-9.9	-10.5	-12.6
2-(6-hydroxy-3-oxo-(3H)-xanthen-9-yl)benzoic acid	700-492-3	1207628-34-9	1207628349	1720	Reach_4912	3509	197	76.3	1.4E-01	1.5E+04	3.5E+00	0		1.1E-06	3.5E-07	1.1E-06				15%	-9.7	-10.5	-12.3
perfluoroethane	200-004-4	50-03-3	50033	2995	Reach_3	3510	405	217.3	2.9E-11	1.2E+02	2.3E+02			3.5E-06	3.5E-07	1.1E-06				23%	-10.9	-10.5	-13.2
3-methylpentan-2-one	222-102-6	3349-08-4	3349084	5580	Reach_1951	3511	205	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				15%	-10.8	-10.5	-12.2
colchicine	200-598-5	64-86-8	64868	782	Reach_75	3512	399	241.8	4.2E-09	1.4E+01	7.2E+01	14.6	15	2.1E-07	1.1E-07	3.5E-07				17%	-9.8	-10.5	-12.2
allyl heptanoate	205-527-1	142-19-8	142198	1950	Reach_1174	3513	170	-10.8	3.0E+01	1.0E+02	4.7E+03			3.5E-06	3.5E-07	1.1E-06				15%	-10.8	-10.5	-12.5
methyl p-toluate	202-784-1	99-75-2	99752	4215	Reach_537	3514	150	5.8	1.4E+01	1.1E+03	2.4E+02			1.1E-06	1.1E-07	3.5E-07				15%	-10.7	-10.5	-12.0
boldenone	212-686-0	846-48-0	846480	3873	Reach_1566	3515	286	145.4	1.6E-06	7.0E+01	1.1E+03	16		1.1E-06	3.5E-07	1.1E-06				15%	-9.8	-10.5	-12.3
2-phenylethyl 2-cyanoacrylate	633-172-6	66415-55-2	66415552	3472	Reach_4600	3516	101	-29.4	1.1E+03	1.0E+06	8.5E-01			1.1E-06	3.5E-07	1.1E-06				15%	-10.7	-10.5	-12.4
(6α,9β,11β,16α)-6-fluoro-17-hydroxy-16-methyl-3,20-dioxo-9,1	700-111-0	148528-05-6	148528056	2002	Reach_4767	3517	158	40.0	4.8E+00	2.4E+03	5.6E+01	0		1.1E-06	1.1E-07	3.5E-07				15%	-9.7	-10.5	-12.3
[4-(2-chloroethoxy)phenyl](phenyl)methanone	613-733-1	64987-06-0	64987060	3447	Reach_4386	3518	200	176.8	8.0E-06	4.4E+04	1.2E+00			3.5E-06	3.5E-07	1.1E-06				16%	-10.7	-10.5	-12.4
3,3'-[methylenebis(oxymethylene)]bisheptane	700-823-1	55514-22-2	55514222	3171	Reach_5002	3519	541	349.8	9.4E-19	1.2E-06	2.6E+06			3.5E-07	1.1E-08	3.5E-08				22%	-10.7	-10.5	-11.9
1,3,5-triisopropylbenzene	231-472-8	7575-23-7	7575237	3684	Reach_2261	3520	489	197.8	6.4E-09	2.1E+01	3.9E+02			3.5E-06	3.5E-07	1.1E-06				23%	-10.8	-10.5	-13.0
trimethylsilyl undec-10-enoate	606-964-4	222408-90-4	222408904	2324	Reach_4230	3521	346	207.9	5.8E-10	1.4E+02	5.4E+02			3.5E-07	3.5E-08	1.1E-07				22%	-10.7	-10.5	-12.5
pentan-2-one	203-528-1	107-87-9	107879	223	Reach_717	3522	86	-67.7	5.3E+03	2.3E+04	5.6E+00			9.4E-07	3.5E-07	1.1E-06				15%	-10.8	-10.5	-12.1
3,4,5-trimethoxybenzoic acid	202-000-8	90-51-7	90517	4001	Reach_365	3523	239	198.1	3.3E-09	1.2E+04	4.1E-02	0.14		1.1E-06	1.1E-07	1.1E-06				14%	-9.7	-10.5	-12.6
1,2,2,6,6-pentamethylpiperidin-4-ol	201-879-5	89-05-4	89054	3968	Reach_338	3524	254	220.2	2.4E-09	1.1E+04	1.4E+00	1.88	0	3.5E-06	3.5E-07	1.1E-06				14%	-10.7	-10.5	-12.4
decyl methacrylate	221-657-1	3179-47-3	3179473	2635	Reach_1927	3525	226	24.1	9.1E-01	2.4E+00	5.0E+05			1.1E-06	1.1E-07	3.5E-07				19%	-10.8	-10.5	-12.3
N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfa	601-485-7	117570-93-1	117570931	1660	Reach_4090	3526	300	204.4	1.3E-07	7.5E+00	1.9E+03	3.63		3.5E-06	3.5E-07	1.1E-06				16%	-9.7	-10.5	-12.3
Benzyl N-(2-benzylacryloyl)glycinate	700-731-1	35958-64-6	35958646	2755	Reach_4980	3527	451	248.4	1.0E-13	1.9E+00	8.5E+02	12.1		3.5E-07	3.5E-08	1.1E-07				15%	-9.9	-10.5	-12.4
diethyl diallylmalonate	262-475-2	60857-05-8	60857058	3318	Reach_2847	3528	152	-20.7	8.4E+01	1.2E+03	3.7E+03			1.1E-06	1.1E-07	3.5E-07				15%	-10.8	-10.5	-12.3
Dilithium naphthalene-1,5-disulfonate	700-037-9	152845-00-6	152845006	5712	Reach_4734	3529	300	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-10.2	-10.5	-12.2
butamirate	230-467-8	7148-78-9	7148789	3583	Reach_2227	3530	206	22.6	8.1E-01	6.9E+02	1.5E+03		0	1.1E-06	1.1E-07	3.5E-07				15%	-10.8	-10.5	-12.4
1,1,2,3,3-pentamethylindan	607-173-7	22871-58-5	22871585	2340	Reach_4234	3531	602	274.7	3.2E-15	1.7E-01	4.0E+01			3.5E-06	3.5E-07	1.1E-06				22%	-10.8	-10.5	-12.6
619-422-7	217-504-3	1874-83-5	1874835	5750	Reach_1729	3532	134	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				16%	-10.8	-10.5	-12.6
(4,5-dibromo-1H-pyrrol-2-yl)(phenyl)methanone	211-490-2	652-37-9	652379	3448	Reach_1487	3533	238	218.8	1.4E-08	2.9E+06	4.6E-02	3.62		1.1E-06	1.1E-07	3.5E-07				15%	-10.7	-10.5	-12.4
3,3'-[biphenyl-4,4'-diylbis(oxy)]dianiline	700-102-1	105112-76-3	105112763	1409	Reach_4764	3534	368	241.7	4.2E-10	6.0E-02	1.1E+06		9.67	1.1E-06	1.1E-07	3.5E-07				15%	-9.9	-10.5	-12.4
2-methylpent-2-enal	696-106-5	1176987-11-3	1176987113	5616	Reach_4704	3535	263	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				14%	-10.8	-10.5	-12.1
dioctylamine	214-311-6	1120-48-5	1120485	1570	Reach_1658	3536	241	57.1	2.4E-01	1.8E-01	5.0E+06		3.1	1.1E-06	1.1E-07	3.5E-07				21%	-10.7	-10.5	-12.7
(2-isobutyl-2-methyl-1,3-dioxolan-4-yl)methanol	616-639-9	78620-07-2	78620072	6037	Reach_4441	3537	222	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				15%	-10.7	-10.5	-12.4
4-[2-(Dimethylamino)-1-(1-hydroxycyclohexyl)ethyl]phenol	700-299-4	2896-97-1	2896971	2551	Reach_4850	3538	300	197.8	3.5E-07	2.5E+01	2.8E+04	12.9	15.1	1.1E-07	3.5E-08	1.1E-07				14%	-9.7	-10.6	-12.4
Tetrasodium {3,3',3'',3'''-[(29H,31H-phthalocyanine-1,8,15,22-t	696-145-8	944730-39-6	944730396	6091	Reach_4707	3539	1373	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-10.2	-10.6	-12.2
allyl 2-hydroxy-2-methylpropanoate	700-908-3	19444-21-4	19444214	2233	Reach_5024	3540	144	-2.2	2.0E+01	9.9E+04	4.3E+00	12.6		3.5E-06	3.5E-07	1.1E-06				14%	-10.8	-10.6	-12.5
3-hydroxy-4-[(2-methyl-4-nitrophenyl)azo]-N-(o-tolyl)naphthal	211-383-0	642-31-9	642319	3431	Reach_1479	3541	206	116.2	7.7E-04	3.4E+01	1.1E+04	0		3.5E-07	1.1E-08	3.5E-08				23%	-10.4	-10.6	-11.3
3-methoxyoestra-1,3,5(10)-trien-17-one	217-968-7	2022-85-7	2022857	2255	Reach_1745	3542	129	94.5	6.0E-04	4.9E+03	3.9E-02			3.5E-07	1.1E-07	3.5E-07				16%	-10.8	-10.6	-12.4
601-431-2	700-505-2	37486-69-4	37486694	2799	Reach_4914	3543	950	100.8	1.8E-02	1.1E-10	1.6E+12			3.5E-07	1.1E-07	3.5E-07				17%	-10.6	-10.6	-12.3
L-cysteine	200-158-2	52-90-4	52904	3080	Reach_18	3544	121	199.3	9.0E-05	8.0E+04	8.9E-04	2	5.55	3.5E-06	3.5E-07	1.1E-06				14%	-9.3	-10.6	-12.6
3-hydroxybenzaldehyde	604-453-0	145022-45-3	145022453	5700	Reach_4154	3545	208	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-10.7	-10.6	-12.4
607-977-8	607-985-1	26678-02-4	26678024	2483	Reach_4257	3546	318	82.0	1.4E-06	7.3E+03	6.2E+02			1.1E-06	1.1E-07	3.5E-07				23%	-10.8	-10.6	-13.3
2-methylbutyl acrylate	256-170-3	44914-03-6	44914036	2934	Reach_2755	3547	142	-45.3	4.1E+02	1.6E+03	4.2E+02			3.5E-06	3.5E-07	1.1E-06				14%	-10.8	-10.6	-12.5
2-Methyloctane-1,8-diamine	700-023-2	130198-05-9	130198059	5658	Reach_4118	3548	286	0.0	0.0E+00	0.0E+00	0.0E+00		0	0.0E+00	0.0E+00	0.0E+00				14%	-10.8	-10.6	-12.4
610-141-5	610-141-5	437717-43-6	437717436	2915	Reach_4322	3549	392	317.1	1.1E-18	1.2E+01	3.2E+00	0.6	5.71	3.5E-07	1.1E-07	3.5E-07				16%	-9.5	-10.6	-12.4
N-phenylacrylamide	606-936-1	2210-24-4	2210244	2318	Reach_4225	3550	147	91.3	2.8E-02	7.9E+02	2.8E+01	15.1	14.4	1.1E-06	3.5E-07	1.1E-06				14%	-10.6	-10.6	-12.5
5-amino-2-(p-aminoanilino)benzenesulphonic acid	700-101-6	246035-38-1	246035381	2399	Reach_4763	3551	408	246.3	2.1E-10	7.2E-01	8.1E+03	0	10.7	1.1E-06	3.5E-08	1.1E-07				14%	-9.3	-10.6	-12.6
tert-butyl 4-(6-aminopyridin-3-yl)piperazine-1-carboxylate	695-268-4	571188-59-5	571188595	3224	Reach_4691	3552	278	160.8	8.2E-05	1.1E+03	9.5E+01		7.63	3.5E-07	3.5E-08	3.5E-07				16%	-9.9	-10.6	-12.4
ethyl (2Z)-4,4,4-trifluoro-3-(methylamino)but-2-enoate	687-796-9	1254333-41-9	1254333419	5642	Reach_4639	3553	1044	0.0	0.0E+00	0.0E+00	0.0E+00		0	0.0E+00	0.0E+00	0.0E+00				14%	-10.8	-10.6	-12.5
N-{6-[3-tert-butyl-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-:	805-439-9	1132935-63-7	1132935637	1615	Reach_5065	3554	494	349.6	1.3E-17	2.6E-03	1.9E+04	8.58		3.5E-07	3.5E-08	1.1E-07				17%	-9.9	-10.6	-12.3
5-aminosalicylic acid	299-135-8	93857-00-2	93857002	6085	Reach_3002	3555	236	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				14%	-9.6	-10.6	-12.6
603-982-4	603-982-4	136890-21-6	136890216	1904	Reach_4136	3556	353	188.2	1.6E-09	5.9E-02	2.6E+07	13		1.1E-06	1.1E-07	3.5E-07				22%	-10.1	-10.6	-11.6
1,2,3,4-tetrahydro-1,1,2,4,4,7-hexamethylnaphthalene	619-692-6	156366-26-6	156366266	2047	Reach_4536	3557	432	226.7	4.3E-09	4.0E+00	1.1E+04			1.1E-06	1.1E-07	3.5E-07				22%	-10.8	-10.6	-12.3
(3,3-diethoxy-1-propenyl)benzene	204-333-4	119-56-2	119562	1695	Reach_980	3558	219	92.5	9.8E-04	2.6E+01	2.2E+03			3.5E-07	1.1E-07	1.1E-07				15%	-10.8	-10.6	-12.4
611-631-1	611-631-1	58190-57-1	58190571	3242	Reach_4363	3559	273	14.1	2.4E-01	4.3E+00	7.1E+08			3.5E-07	1.1E-07	3.5E-07				23%	-10.4	-10.6	-11.4
1-(2-chloroethoxy)-4-(1,2-diphenylvinyl)benzene	700-227-1	40722-73-4	40722734	2862	Reach_4812	3560	218	64.3	2.3E-01	8.2E+03	7.6E+00			3.5E-07	1.1E-07	3.5E-07				21%	-10.4	-10.6	-11.9
2-hexyldecyl methanesulfonate	212-985-6	901-44-0	901440	3991	Reach_1588	3561	316	175.3	7.5E-09	1.3E+03	1.7E+03			3.5E-07	3.5E-08	1.1E-07				19%	-10.9	-10.6	-13.1
615-927-1	609-206-0	361366-16-7	361366167	2759	Reach_4294	3562	359	108.6	3.6E-04	7.7E-01	4.3E+05			1.1E-06	1.1E-07	3.5E-07				16%	-10.9	-10.6	-12.7
trimethylsilyl N-trimethylsilylacetamidate	225-063-3	4637-24-5	4637245	2953	Reach_2052	3563	119	-58.2	3.7E+03	4.9E+05	3.1E-01		9.3	1.1E-06	1.1E-07	3.5E-07				21%	-10.9	-10.6	-13.5
ethyl N-(diphenylmethylidene)glycinate	614-987-6	69555-14-2	69555142	3544	Reach_4405	3564	267	94.2	1.4E-03	1.3E+01	6.5E+03		9.62	1.1E-06	1.1E-07	3.5E-07				14%	-10.1	-10.6	-12.6
phenyl diamidophosphate	231-218-6	7450-69-3	7450693	3638	Reach_2251	3565	172	70.1	7.0E-02	9.9E+04	1.7E-01			1.1E-06	1.1E-07	3.5E-07				14%	-9.7	-10.6	-12.8
1-methylhexyl chloroacetate	606-870-3	219715-34-1	219715341	2312	Reach_4222	3566	177	7.8	2.5E+02	1.2E+03	2.0E+02			3.5E-07	3.5E-08	1.1E-07				15%	-10.9	-10.6	-12.3
3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulphonyl chloride	610-147-8	438056-69-0	438056690	2917	Reach_4323	3567	192	139.2	4.1E-04	1.5E+04	4.2E-01			1.1E-06	1.1E-07	1.1E-06				22%	-10.8	-10.6	-13.5
benzyl (4-bromo-3-fluorophenyl)carbamate	265-250-7	64838-55-7	64838557	3444	Reach_2867	3568	259	159.8	2.9E-05	8.4E+03	1.9E+00	3.28		3.5E-06	3.5E-07	1.1E-06				17%	-10.8	-10.6	-12.4
tert-pentyl 2-ethylperoxyhexanoate	211-687-3	686-31-7	686317	3523	Reach_1502	3569	230	25.3	2.7E+00	5.1E-02	6.3E+04			3.5E-07	1.1E-07	3.5E-07				23%	-10.9	-10.6	-13.4
1,1,1,2,4,4,5,7,7,8,10,10,11,13,13,14,16,16,17,17,18,18,18-tric	228-771-0	6358-37-8	6358378	3408	Reach_2169	3570	658	349.8	2.7E-20	1.4E-05	1.4E+08			3.5E-07	3.5E-08	3.5E-08				24%	-10.9	-10.6	-11.5
diethyl (phenylmethylene)malonate	266-330-4	66356-53-4	66356534	3470	Reach_2878	3571	214	86.3	4.5E-02	4.1E+04	5.9E+00			1.1E-06	1.1E-07	3.5E-07				15%	-10.9	-10.6	-12.4
but-3-enenitrile	203-701-1	109-75-1	109751	264	Reach_789	3572	67	-59.8	2.2E+03	3.6E+04	5.0E+00			8.1E-07	1.1E-07	3.5E-07				15%	-10.9	-10.6	-12.0
O-(2-ethylhexyl) O,O-tert-pentyl peroxycarbonate	274-919-2	70833-40-8	70833408	3570	Reach_2921	3573	260	5.8	2.6E-01	1.3E+00	1.4E+05			1.1E-06	1.1E-07	3.5E-07				18%	-10.9	-10.6	-12.3
ethyl 2-methylvalerate	204-688-5	124-19-6	124196	1788	Reach_1073	3574	142	-19.5	7.5E+01	1.5E+02	1.9E+03			3.5E-07	3.5E-08	1.1E-07				15%	-10.9	-10.6	-12.6
4-[(4,6-Bis{[3-(diethylamino)propyl]amino}-1,3,5-triazin-2-yl)an	700-650-1	909782-35-0	909782350	4010	Reach_4959	3575	917	349.8	1.5E-24	9.2E-09	1.7E+10	9.35	2.9	1.1E-07	1.1E-07	1.1E-07				24%	-10.7	-10.6	-11.2
myristoyl chloride	800-308-2	1160221-25-9	1160221259	1641	Reach_5044	3576	509	267.0	8.0E-12	3.1E-03	2.4E+08			1.1E-06	1.1E-07	3.5E-07				21%	-10.9	-10.6	-13.3
3-(9,10-ethano-9(10H)-anthryl)acrylaldehyde	226-529-9	5419-55-6	5419556	3131	Reach_2108	3577	188	-43.0	1.1E+03	0.0E+00	6.8E+00			1.1E-06	3.5E-07	1.1E-06				15%	-10.9	-10.6	-12.5

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
601-507-5	226-845-7	5505-16-8	5505168	3158	Reach_2119	3578	530	213.0	3.5E-08	4.9E+00	7.8E+01			1.1E-06	1.1E-07	3.5E-07				21%	-10.9	-10.6	-13.5
ethyl [(1-chloro-10-oxo-10H-dibenzo[b,e]thiopyran-4-yl)oxy]ac	700-766-2	61010-04-6	61010046	3323	Reach_4988	3579	173	73.8	7.2E-03	8.2E+03	7.9E+01			1.1E-06	3.5E-07	1.1E-06				17%	-10.4	-10.6	-12.4
icosanoic acid	209-935-0	598-50-5	598505	3289	Reach_1402	3580	74	11.0	2.3E+01	3.7E+05	8.1E-02	14.3		3.5E-07	1.1E-07	1.1E-06				20%	-10.7	-10.6	-12.0
1-(2-ethylbutyl)cyclohexanecarbonyl chloride	259-515-6	55184-72-0	55184720	5929	Reach_2806	3581	585	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				22%	-10.9	-10.6	-13.3
608-211-5	608-211-5	284462-37-9	284462379	2532	Reach_4265	3582	243	189.3	1.2E-06	2.5E+03	6.3E+01	14.8	9.07	1.1E-06	1.1E-07	3.5E-07				14%	-9.8	-10.6	-12.7
N,N'-[cyclohexane-1,3-diylbis(methylene)]bis(2-methylpropan-	619-764-7	173904-11-5	173904115	2133	Reach_4543	3583	250	14.7	2.0E-01	8.4E+00	1.3E+05		6.8	3.5E-07	1.1E-07	3.5E-07				19%	-10.9	-10.6	-11.8
614-960-9	614-960-9	69399-57-1	69399571	3542	Reach_4403	3584	237	214.4	2.8E-08	5.9E+03	1.6E+00	4.71		3.5E-06	1.1E-07	3.5E-07				14%	-9.4	-10.6	-12.8
(4S)-4-(phenylthio)-L-proline	202-215-7	93-07-2	93072	4058	Reach_398	3585	182	95.7	3.1E-03	3.5E+03	3.3E+01	4.28	0	1.1E-06	3.5E-07	1.1E-06				14%	-9.4	-10.6	-12.7
3-nitro-p-anisic acid	201-906-0	89-41-8	89418	3975	Reach_343	3586	197	128.7	1.8E-03	1.1E+03	5.9E+01	3.66		3.5E-06	1.1E-07	3.5E-07				14%	-9.8	-10.6	-12.8
benzimidazole-2-thiol	200-984-3	76-75-5	76755	877	Reach_177	3587	242	215.8	2.3E-08	4.3E+01	2.2E+02	7.5	0	2.6E-07	3.5E-07	1.1E-06				14%	-9.8	-10.7	-12.7
calcium bis{4-[(E)-(5-carbamoyl-2-methoxyphenyl)diazenyl]-3-h	700-038-4	17273-79-9	17273799	5739	Reach_4735	3588	194	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-10.3	-10.7	-12.3
604-604-0	252-677-9	35689-59-9	35689599	5857	Reach_2693	3589	663	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				19%	-10.1	-10.7	-12.3
Ethyl 3-cyclobutylalaninate	227-086-4	5638-76-6	5638766	3195	Reach_2130	3590	136	27.9	1.8E+01	5.6E+02	3.0E+00		4.2	3.5E-07	3.5E-08	1.1E-07				14%	-10.8	-10.7	-12.6
5-chlorothiophene-2-sulfonamide	805-591-6	210223-97-5	210223975	5770	Reach_5066	3591	303	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				16%	-9.9	-10.7	-12.6
806-599-2	680-297-7	88110-89-8	88110898	3947	Reach_4624	3592	481	349.8	2.0E-20	1.0E+03	1.6E+00			3.5E-07	3.5E-08	3.5E-07				17%	-10.1	-10.7	-12.4
Sodium naphthalene-2-carboxylate	700-756-8	1204232-63-2	1204232632	5626	Reach_4986	3593	769	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-10.4	-10.7	-12.3
1-{[(methylsulfanyl)carbonyl]oxy}ethyl 2-methylpropanoate	700-047-3	860035-07-0	860035070	3899	Reach_4739	3594	192	-62.4	4.3E+01	8.0E+03	1.9E+00			3.5E-06	3.5E-07	1.1E-06				14%	-10.9	-10.7	-12.5
610-977-0	700-391-4	6953-28-2	6953282	6003	Reach_4885	3595	245	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				18%	-9.9	-10.7	-12.3
1-(1,1-dimethylethoxy)-2-methylpropane	212-811-9	871-78-3	871783	3920	Reach_1577	3596	144	141.6	5.3E-04	4.7E+05	1.9E-02			3.5E-06	3.5E-07	1.1E-06				20%	-11.0	-10.7	-13.6
3-(2-(2-Hydroxyethoxy)ethylimino)-2,2-dimethylpropyldodecar	700-067-2	931419-77-1	931419771	4062	Reach_4748	3597	372	158.8	1.1E-07	1.8E-01	1.1E+05	14.9	8.56	1.1E-06	1.1E-07	3.5E-07				15%	-10.0	-10.7	-12.5
methyl 3-oxohexanoate	213-493-4	959-14-8	959148	4137	Reach_1618	3598	245	132.0	1.2E-02	7.9E+02	2.3E+02	0		3.5E-07	3.5E-08	1.1E-07				14%	-10.9	-10.7	-12.3
(2S,3S,5R)-3-methyl-7-oxo-3-(1H-1,2,3-triazol-1-ylmethyl)-4-thi	618-303-7	89786-04-9	89786049	3986	Reach_4492	3599	300	212.6	3.7E-08	3.4E+05	1.9E-02	2.41	13.5	3.5E-06	3.5E-07	1.1E-06				14%	-9.4	-10.7	-12.7
610-200-5	700-255-4	31775-89-0	31775890	2633	Reach_4825	3600	545	195.7	2.3E-09	8.5E-01	1.8E+04	8.95	0	1.1E-06	1.1E-07	1.1E-06				14%	-9.5	-10.7	-12.7
diisopentyl ether	208-857-4	544-01-4	544014	3141	Reach_1351	3601	158	-49.1	2.5E+02	3.4E+01	7.1E+03			1.1E-06	1.1E-07	3.5E-07				20%	-11.0	-10.7	-13.4
619-847-8	619-847-8	111298-82-9	111298829	1546	Reach_4550	3602	401	332.3	3.7E-14	2.7E+01	5.5E-01	2.48	7.03	3.5E-07	1.1E-07	3.5E-07				16%	-9.6	-10.7	-12.6
N-(5-chloro-2,4-dimethoxyphenyl)-4-[[5-[(diethylamino)sulpho	229-107-2	6410-41-9	6410419	3425	Reach_2179	3603	627	349.8	3.5E-20	4.6E-04	4.5E+07	9.27		1.1E-06	3.5E-08	1.1E-07				22%	-10.3	-10.7	-11.8
methyl hexanoate	239-263-3	15206-55-0	15206550	2020	Reach_2377	3604	164	34.9	2.7E+00	5.0E+03	3.1E+01			3.5E-06	3.5E-07	1.1E-06				14%	-11.0	-10.7	-12.6
octafluoropropane	200-941-9	76-19-7	76197	3702	Reach_174	3605	188	-136.4	7.1E+05	3.7E+00	6.6E+02			3.5E-08	1.1E-08	3.5E-08				23%	-11.0	-10.7	-13.4
N-(4-{[3-(dimethylamino)propyl]sulfamoyl}phenyl)-2-[(2-metho	700-222-4	1065519-44-9	1065519449	1438	Reach_4809	3606	521	311.4	6.7E-15	3.0E+00	1.6E+03	8.32	3.15	3.5E-07	3.5E-08	1.1E-07				16%	-9.9	-10.7	-12.5
607-088-5	607-088-5	224785-90-4	224785904	2334	Reach_4232	3607	489	342.0	4.6E-17	2.9E+01	6.2E+02		5.93	3.5E-07	1.1E-07	3.5E-07				16%	-10.0	-10.7	-12.5
bis(2-propylheptyl) carbonate	700-195-9	223398-24-1	223398241	5782	Reach_4800	3608	307	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				23%	-10.6	-10.7	-12.1
cyclopentene	700-377-8	99817-37-5	99817375	4217	Reach_4882	3609	206	112.6	3.1E-03	1.2E+02	8.3E+02			1.1E-06	3.5E-08	1.1E-07				20%	-11.0	-10.7	-13.6
2,3-Dihydro-1,4-benzodioxin-2-yl(piperazin-1-yl)methanone	685-040-2	81778-06-5	81778065	3812	Reach_4629	3610	152	102.9	5.4E-04	2.9E+04	2.1E+00		0	3.5E-07	1.1E-07	3.5E-07				14%	-9.7	-10.7	-12.8
6-[3-tert-butyl-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-2-m	695-991-5	1355646-97-7	1355646977	1890	Reach_4700	3611	699	344.5	3.0E-17	4.4E-07	4.3E+08	9.68		3.5E-07	3.5E-08	1.1E-07				23%	-10.5	-10.7	-11.4
menthyl acetate	201-911-8	89-48-5	89485	3976	Reach_344	3612	198	0.7	1.2E+01	1.6E+02	2.5E+04			3.5E-06	3.5E-07	1.1E-06				16%	-11.0	-10.7	-12.4
2-ethylhexyl nonanoate	700-472-4	27665-39-0	27665390	2514	Reach_4906	3613	218	160.6	1.3E-07	2.2E+05	1.2E-02			1.1E-06	1.1E-07	3.5E-07				22%	-10.8	-10.7	-12.6
methyl L-threoninate	608-135-2	27710-82-3	27710823	5811	Reach_4261	3614	509	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				14%	-10.2	-10.7	-12.9
3,5-bis(2,4-dimethylcyclohex-3-en-1-yl)dihydro-1H-[1,3]oxazolo	700-437-3	1196069-20-1	1196069201	1696	Reach_4899	3615	332	147.4	7.7E-05	2.5E+01	6.0E+06		7.55	1.1E-06	1.1E-07	3.5E-07				20%	-10.5	-10.7	-12.3
ethyl trichloroacetate	208-212-7	515-84-4	515844	3042	Reach_1320	3616	191	-10.6	2.3E+02	1.2E+03	1.7E+02			3.5E-06	3.5E-07	1.1E-06				14%	-11.0	-10.7	-12.7
1-(2,4-dichloro-5-fluorophenyl)ethanone	256-127-9	43170-88-3	43170883	2906	Reach_2754	3617	511	317.1	2.6E-15	3.7E+00	7.2E+00			1.1E-06	1.1E-07	3.5E-07				19%	-11.0	-10.7	-12.1
1-chlorohexane	245-485-1	23202-81-5	23202815	2347	Reach_2528	3618	188	31.6	1.7E+01	1.2E+04	3.0E+00			3.5E-07	1.1E-07	3.5E-07				20%	-11.0	-10.7	-13.5
diisopentyl phthalate	678-536-5	52698-46-1	52698461	3070	Reach_4619	3619	148	-43.6	1.5E+03	3.8E+03	1.1E+02			1.1E-06	1.1E-07	1.1E-06				18%	-10.3	-10.7	-12.4
tetrachloro-1,2-difluoroethane	200-935-6	76-12-0	76120	3700	Reach_172	3620	204	-49.5	6.3E+03	1.1E+02	2.6E+03			3.5E-08	1.1E-08	1.1E-08				23%	-11.2	-10.7	-13.4
trifluoroacetic anhydride	206-982-9	407-25-0	407250	2863	Reach_1267	3621	210	-101.8	5.9E+04	6.9E-01	1.8E+00			3.5E-06	3.5E-07	1.1E-06				17%	-11.0	-10.7	-14.0
5-amino-3-methylthiophene-2,4-dicarbonitrile	269-389-4	68227-78-1	68227781	3512	Reach_2902	3622	565	349.8	1.1E-20	1.3E-04	5.1E+08			1.1E-07	3.5E-09	1.1E-08				14%	-10.0	-10.7	-12.8
N-(2-Bromo-5-hydroxy-4-methoxybenzyl)-N-[2-(4-hydroxypher	602-791-3	122584-18-3	122584183	1753	Reach_4105	3623	380	211.6	9.3E-10	6.9E-02	5.4E+02	9.31	14.4	1.1E-06	1.1E-07	3.5E-07				15%	-10.0	-10.7	-12.7
(3R)-3-[2-(Benzyloxy)-5-bromophenyl]-N,N-diisopropyl-3-phen	604-958-6	15448-47-2	15448472	489	Reach_4165	3624	58	-100.2	7.1E+04	5.8E+04	2.3E+00		0	6.1E-07	1.1E-07	3.5E-07				23%	-10.3	-10.8	-11.5
(2-formamido-1,3-thiazol-4-yl)(oxo)acetic acid	690-635-5	3439-73-4	3439734	2703	Reach_4658	3625	261	119.8	6.3E-04	5.3E+00	9.3E+03	0	0	1.1E-06	3.5E-08	1.1E-07				14%	-9.7	-10.8	-12.8
689-979-9	689-979-9	116817-12-0	116817120	5613	Reach_4655	3626	401	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-10.4	-10.8	-12.4
pentyl propionate	217-775-8	1951-97-9	1951979	5761	Reach_1738	3627	184	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				15%	-11.0	-10.8	-12.7
1-Phenylsulfonylpyrrole	623-685-3	16851-82-4	16851824	2113	Reach_4578	3628	207	109.7	3.7E-03	1.1E+03	1.5E+02		15	1.1E-06	1.1E-07	3.5E-07				14%	-10.0	-10.8	-12.8
(S)-p-mentha-1,8-diene	227-815-6	5989-54-8	5989548	744	Reach_2148	3629	136	-40.8	1.9E+02	7.7E+00	6.8E+04			5.7E-07	1.1E-07	3.5E-07				22%	-11.1	-10.8	-13.5
triacetoxyvinylsilane	223-943-1	4130-08-9	4130089	1265	Reach_2015	3630	232	-35.0	1.1E+01	0.0E+00	4.0E+00			3.5E-06	3.5E-07	1.1E-06				14%	-10.8	-10.8	-12.8
2-chloro-1-(3,4-difluorophenyl)ethanone	607-988-8	2668-75-9	2668759	2484	Reach_4258	3631	368	185.7	2.1E-06	2.4E+01	1.7E+03			1.1E-06	3.5E-07	1.1E-06				15%	-11.0	-10.8	-12.3
(Z)-hex-3-enyl acetate	222-960-1	3681-71-8	3681718	2779	Reach_1979	3632	142	-33.3	1.5E+02	6.9E+02	4.1E+02			3.5E-06	3.5E-07	1.1E-06				14%	-11.1	-10.8	-12.6
1-[3-tert-butyl-5-(6-hydroxy-2-naphthyl)-4-methoxyphenyl]pyr	805-127-2	1355646-93-3	1355646933	1889	Reach_5061	3633	416	301.8	1.5E-15	1.3E-02	3.5E+05	9.43		3.5E-07	3.5E-08	1.1E-07				20%	-10.0	-10.8	-12.3
1-(benzyloxy)-4-[2-(cyclopropylmethoxy)ethyl]benzene	613-114-6	62932-92-7	62932927	3388	Reach_4381	3634	231	120.9	3.1E-04	5.3E+03	1.1E+01			3.5E-06	3.5E-07	1.1E-06				18%	-10.9	-10.8	-12.5
602-769-3	700-172-3	634-55-9	634559	3402	Reach_4789	3635	155	36.2	2.3E+00	4.2E+03	1.0E-01	7.8		3.5E-06	3.5E-07	1.1E-06				14%	-9.7	-10.8	-12.9
thiocolchicine	220-346-8	2730-71-4	2730714	2499	Reach_1859	3636	416	251.7	8.9E-11	3.7E+00	3.2E+02	14.6	14.7	3.5E-07	1.1E-07	3.5E-07				16%	-10.2	-10.8	-12.6
3-amino-4-hydroxybenzenesulphonic acid	256-442-1	49715-04-0	49715040	2988	Reach_2764	3637	165	40.4	6.9E+00	1.8E+04	9.3E+01	0	0	3.5E-06	1.1E-06	3.5E-06				14%	-9.6	-10.8	-13.1
1,1,3,3-tetramethylbutyl 2-ethylperoxyhexanoate	244-894-2	22288-43-3	22288433	2328	Reach_2521	3638	272	52.9	2.7E-01	4.2E-01	1.4E+06			3.5E-07	1.1E-07	3.5E-07				22%	-11.0	-10.8	-12.7
L-leucine	700-811-6	87428-99-7	87428997	3934	Reach_5000	3639	309	193.5	3.5E-07	1.1E+00	4.6E+03	12.8	0	1.1E-06	1.1E-07	3.5E-07				14%	-9.5	-10.8	-12.8
2,2-Dimethyl-3-(morpholin-4-yl)propanal	700-569-1	23588-51-4	23588514	2352	Reach_4937	3640	171	41.1	4.7E+00	1.8E+05	1.0E+00		7.5	1.1E-06	1.1E-07	3.5E-07				14%	-10.3	-10.8	-12.9
5-methylisoxazole-4-carboxylic acid	700-843-0	198979-98-5	198979985	6399	Reach_5008	3641	1071	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-9.8	-10.8	-12.8
Cyclopropane-1,1-diyldimethanol	700-582-2	30392-50-8	30392508	5831	Reach_4939	3642	384	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-10.3	-10.8	-12.9
(R)-quinuclidin-3-ol	610-977-0	53201-62-0	53201620	3090	Reach_4342	3643	350	197.2	3.7E-09	8.4E+00	1.3E+05	8.19	0	1.1E-06	1.1E-07	3.5E-07				14%	-9.8	-10.8	-12.9
piperidine-2-methylamine	700-696-2	1062580-52-2	1062580522	5597	Reach_4971	3644	291	0.0	0.0E+00	0.0E+00	0.0E+00		0	0.0E+00	0.0E+00	0.0E+00				14%	-10.8	-10.8	-12.9
4-methoxybenzyl (6R,7R)-7-amino-3-(chloromethyl)-8-oxo-5-th	800-008-1	21524-36-7	21524367	2296	Reach_5034	3645	219	77.3	5.1E-02	2.5E+00	2.8E+05	0	9.1	3.5E-07	3.5E-08	1.1E-07				14%	-9.6	-10.8	-12.9
N-(2-ethylhexyl)isononan-1-amide	806-533-2	1219086-87-9	1219086879	1738	Reach_5075	3646	310	128.8	3.0E-04	1.3E-01	3.4E+05	0	0	1.1E-08	3.5E-09	1.1E-08				21%	-10.9	-10.8	-12.1
(5,6-Dimethyl-9-oxo-9H-xanthen-4-yl)acetic acid	696-006-1	123348-27-6	123348276	1769	Reach_4703	3647	371	134.1	2.8E-04	1.2E-02	1.2E+06	0	0	1.1E-07	1.1E-08	3.5E-08				14%	-10.2	-10.8	-12.8
609-736-2	204-975-5	130-13-2	130132	5657	Reach_1116	3648	245	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				15%	-9.9	-10.8	-12.7
2-methylquinoline-4-carboxamide	239-917-8	15821-13-3	15821133	2058	Reach_2400	3649	186	155.6	1.1E-04	2.5E+03	2.7E+01	14.8	11	1.1E-06	1.1E-07	3.5E-07				14%	-10.0	-10.8	-12.9
retinyl acetate	204-844-2	127-47-9	127479	1812	Reach_1098	3650	329	115.0	2.5E-04	3.0E-02	4.3E+08			3.5E-06	3.5E-07	1.1E-06				22%	-10.5	-10.8	-11.7
S-1,3-benzothiazol-2-yl (2Z)-(2-amino-1,3-thiazol-4-yl)[(trityloxy	606-000-2	1836-62-0	1836620	2186	Reach_4189	3651	167	53.8	1.1E+00	1.3E+05	4.6E+00		4.9	1.1E-06	3.5E-07	1.1E-06				17%	-10.2	-10.8	-12.6
2-[3-(9-butyl-1,1,3,3,5,5,7,7,9,9-decamethylpentasiloxanyl)pro	801-072-3	1052075-57-6	1052075576	1411	Reach_5051	3652	583	116.5	7.7E-05	1.6E-06	1.7E+12			3.5E-06	3.5E-07	1.1E-06				24%	-11.1	-10.8	-11.6

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
610-201-0	610-200-5	446292-07-5	446292075	2929	Reach_4326	3653	395	294.3	8.2E-17	6.2E+02	1.9E+00		10.2	1.1E-06	1.1E-07	3.5E-07				14%	-9.9	-10.8	-12.8
3-Hydroxy-2,2-dimethyl-N-propylpropanamide	219-351-8	2422-91-5	2422915	2380	Reach_1804	3654	367	169.5	3.0E-06	9.4E-01	1.5E+07	0	0	1.1E-06	3.5E-07	1.1E-06				14%	-9.7	-10.8	-12.8
2,2,6,6-Tetramethylpiperidin-4-yl dodecanoate	700-503-1	101238-01-1	101238011	1317	Reach_4913	3655	340	146.8	1.2E-04	1.4E-02	7.2E+06		4.4	1.1E-06	1.1E-07	3.5E-07				21%	-10.8	-10.8	-12.2
3-amino-4-methoxybenzenesulphonic acid	609-812-5	402913-84-2	402913842	2856	Reach_4313	3656	695	349.8	6.1E-33	5.7E+01	5.8E-01	7.98	14.3	1.1E-06	1.1E-07	3.5E-07				14%	-9.8	-10.8	-13.0
610-472-5	610-472-5	49707-23-5	49707235	2987	Reach_4329	3657	159	75.1	1.7E-01	4.7E+04	1.1E-01	14	15.3	1.1E-06	3.5E-07	1.1E-06				14%	-9.7	-10.9	-12.8
gestonorone	700-845-1	133978-15-1	133978151	1874	Reach_5009	3658	209	36.3	2.4E-01	4.0E+01	1.9E+04	0		1.1E-06	1.1E-07	3.5E-07				16%	-10.0	-10.9	-12.7
2,5-bis(2,2,2-trifluoroethoxy)benzoic acid	611-756-1	58861-48-6	58861486	3255	Reach_4364	3659	178	61.7	4.0E-01	2.1E+01	6.0E+03	0		1.1E-06	1.1E-07	3.5E-07				14%	-10.1	-10.9	-13.0
(2β,3α,5α,16β,17β)-2-(morpholin-4-yl)-16-(pyrrolidin-1-yl)andr	205-812-0	153-00-4	153004	2027	Reach_1210	3660	302	149.8	1.5E-06	3.5E+01	4.9E+03	16	0	3.5E-07	1.1E-07	3.5E-07				16%	-10.0	-10.9	-12.7
3,3,4,4,5,5,6,6,6-nonafluorohexene	243-053-7	19430-93-4	19430934	2231	Reach_2479	3661	246	-105.8	1.8E+05	4.1E+00	2.5E+04			3.5E-06	3.5E-07	1.1E-06				19%	-11.2	-10.9	-14.2
3-(3,5-di-tert-butyl-4-hydroxyphenyl)-N-octadecylpropanamide	700-596-9	14442-94-5	14442945	1976	Reach_4944	3662	530	273.7	1.9E-13	1.3E-07	2.2E+12	12	14.2	1.1E-06	1.1E-07	3.5E-07				24%	-11.1	-10.9	-11.3
(S)-1-[3-(acetylthio)-2-methyl-1-oxopropyl]-L-proline	609-612-8	3910-51-8	3910518	2834	Reach_4306	3663	212	139.6	3.7E-04	1.1E+02	1.6E+02	13		3.5E-07	3.5E-08	1.1E-07				14%	-9.8	-10.9	-12.9
2,4-dihydroxybenzophenone	205-029-4	131-56-6	131566	1850	Reach_1121	3664	214	141.9	1.9E-05	2.5E+03	9.1E+02	7.83		3.5E-07	1.1E-07	3.5E-07				16%	-10.2	-10.9	-12.6
2-oxopropyl 3-(benzyl-[4-(2-cyano-4-nitrophenylazo)phenyl]am	627-085-2	1238449-42-7	1238449427	1776	Reach_4584	3665	343	9.0	3.5E-03	2.1E-03	8.5E+08		0	1.1E-06	1.1E-07	3.5E-07				14%	-10.3	-10.9	-12.9
1,1,1,2,2,3,3,4,5,5,5-undecafluoro-4-(trifluoromethyl)pentane	206-575-6	355-04-4	355044	2740	Reach_1250	3666	338	-88.9	3.0E+04	2.1E-01	1.0E+05			3.5E-08	1.1E-08	3.5E-08				24%	-11.2	-10.9	-13.5
600-715-3	263-266-9	61832-41-5	61832415	3355	Reach_2851	3667	148	40.3	5.4E+00	2.8E+05	4.8E-01		6.37	3.5E-07	3.5E-08	3.5E-07				14%	-10.0	-10.9	-12.9
609-425-1	609-425-1	374067-80-8	374067808	2797	Reach_4301	3668	228	237.9	2.7E-12	5.8E+01	8.9E+00	6.58	5.1	3.5E-06	3.5E-07	1.1E-06				14%	-9.9	-10.9	-12.9
5-chlorothiophene-2-sulfonyl chloride	700-040-5	674347-28-5	674347285	5985	Reach_4736	3669	178	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				17%	-11.1	-10.9	-12.7
Tetrahydro-2-furancarboxylic acid	700-744-2	99842-68-9	99842689	4220	Reach_4984	3670	189	72.2	4.3E-02	1.5E+03	5.2E+01	0		1.1E-06	1.1E-07	3.5E-07				14%	-9.8	-10.9	-12.9
11β,16α,17,21-tetrahydroxypregna-1,4-diene-3,20-dione	700-400-1	42831-50-5	42831505	2899	Reach_4887	3671	127	65.3	1.9E+00	3.2E+04	4.4E+00	4.8		1.1E-06	1.1E-07	3.5E-07				14%	-10.0	-10.9	-12.8
2-bromo-7-iodo-9H-fluorene	700-338-5	50372-61-7	50372617	3004	Reach_4867	3672	329	138.3	2.7E-04	5.2E+00	6.5E+03			1.1E-06	1.1E-07	3.5E-07				22%	-11.1	-10.9	-12.1
3-amino-4-hydroxybenzenesulphonamide	806-756-5	1262985-24-9	1262985249	1804	Reach_5080	3673	631	303.0	2.6E-14	4.1E-04	9.8E+04	6.51	14.5	3.5E-08	1.1E-08	3.5E-08				14%	-9.7	-10.9	-13.1
2-bromo-1-(3,5-dihydroxyphenyl)ethanone	620-134-9	1172131-64-4	1172131644	1656	Reach_4559	3674	418	253.3	7.0E-11	3.7E+01	3.3E+02	12.6		1.1E-06	1.1E-07	3.5E-07				14%	-10.0	-10.9	-12.9
11β,17,21-trihydroxy-6α-methylpregna-1,4-diene-3,20-dione 2	220-976-3	2955-88-6	2955886	2569	Reach_1892	3675	115	16.8	1.2E+01	4.1E+05	8.5E-01	15		3.5E-06	1.1E-06	3.5E-06				14%	-10.1	-10.9	-12.8
Ethyl 1-(4-methoxyphenyl)-6-(4-nitrophenyl)-7-oxo-4,5,6,7-tetr	611-033-0	536759-91-8	536759918	3108	Reach_4347	3676	436	264.5	1.2E-11	2.7E+00	1.1E+04		14.2	1.1E-06	3.5E-08	1.1E-07				16%	-10.1	-10.9	-12.7
2-pyrrolidin-1-ylethanol	696-003-5	924726-92-1	924726921	4036	Reach_4702	3677	495	241.7	1.3E-12	1.7E-02	3.4E+03	13	0	1.1E-06	1.1E-07	3.5E-07				14%	-10.8	-10.9	-12.9
cis-4-tert-butylcyclohexyl acetate	233-881-7	10411-92-4	10411924	1383	Reach_2290	3678	198	10.9	9.1E+00	4.3E-01	2.6E+04			3.5E-06	3.5E-07	1.1E-06				18%	-11.2	-10.9	-14.1
triisopropyl borate	700-123-6	934985-83-8	934985838	4071	Reach_4770	3679	263	140.1	9.1E-06	6.1E+03	5.2E+02			1.1E-05	1.1E-06	3.5E-06				14%	-11.2	-10.9	-12.5
ethyl phenylacetate	620-345-6	873055-55-1	873055551	3925	Reach_4567	3680	309	131.4	2.6E-04	3.0E+00	1.2E+05			3.5E-07	3.5E-08	1.1E-07				15%	-11.2	-10.9	-12.4
3-oxoglutaric acid	210-155-8	608-25-3	608253	3317	Reach_1414	3681	124	59.6	3.4E-02	2.5E+05	3.8E+01	9.6		1.1E-05	1.1E-06	3.5E-06				14%	-9.7	-10.9	-13.0
Ethyl 2-(3-formyl-4-hydroxyphenyl)-4-methyl-1,3-thiazole-5-car	204-320-3	119-40-4	119404	1691	Reach_977	3682	315	227.7	1.7E-11	2.0E+01	6.8E+00	-0.43	12.4	3.5E-07	3.5E-08	1.1E-07				14%	-10.2	-10.9	-12.9
619-482-4	619-482-4	895525-70-9	895525709	3977	Reach_4522	3683	219	128.2	5.4E-05	3.2E+03	5.0E+00	11.5		3.5E-06	3.5E-07	1.1E-06				14%	-10.0	-10.9	-13.0
labetalol	237-731-1	13951-70-7	13951707	1921	Reach_2353	3684	376	232.2	6.1E-13	6.7E+02	1.1E+01	12.6	0	1.1E-06	3.5E-07	1.1E-06				15%	-10.0	-10.9	-12.8
1,2-dihydro-3H-1,2,4-triazol-3-one	208-835-4	542-92-7	542927	3137	Reach_1348	3685	66	-91.8	5.7E+04	1.7E+03	1.8E+02		0	1.1E-06	1.1E-07	3.5E-07				14%	-9.8	-10.9	-12.9
620-216-4	620-216-4	298692-41-8	298692418	2575	Reach_4561	3686	181	66.8	1.4E-01	7.7E+05	1.2E-02	9.3		3.5E-06	3.5E-07	1.1E-06				14%	-9.9	-10.9	-13.1
benzene-1,2,4,5-tetracarboxylic acid	200-041-6	50-48-6	50486	662	Reach_8	3687	277	134.4	4.8E-05	3.5E+00	8.9E+04	0		2.3E-08	1.1E-08	3.5E-08				14%	-9.8	-10.9	-12.9
5-amino-3-(4-chlorophenyl)-5-oxopentanoic acid	700-677-9	19190-61-5	19190615	2227	Reach_4965	3688	306	-52.6	2.3E+03	7.6E+01	4.5E+02	0	0	3.5E-06	3.5E-07	1.1E-06				14%	-10.0	-10.9	-13.0
4-nitroimidazole	221-224-7	3034-38-6	3034386	2593	Reach_1902	3689	113	94.8	8.6E-05	4.6E+04	7.6E-01	9	13.8	1.1E-06	1.1E-07	3.5E-07				14%	-9.9	-10.9	-13.1
Ethyl 4-oxocyclohexanecarboxylate	601-635-1	119812-29-2	119812292	5624	Reach_4097	3690	293	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				14%	-11.2	-10.9	-12.9
17-hydroxy-19-norpregn-4-ene-3,20-dione 17-acetate	689-732-5	956317-36-5	956317365	4128	Reach_4652	3691	203	153.4	2.4E-04	3.6E+03	6.9E+01			3.5E-06	3.5E-07	1.1E-06				16%	-10.3	-10.9	-12.7
1H-tetrazol-1-acetic acid	244-551-7	21732-17-2	21732172	2304	Reach_2508	3692	128	97.8	1.8E-01	5.5E+04	3.0E-03	4		3.5E-06	3.5E-07	1.1E-06				14%	-9.8	-10.9	-13.0
2-[2-(carboxymethyl)phenoxy]-3,4-dimethylbenzoic acid	941-156-8	1554631-80-9	1554631809	2041	Reach_5180	3693	315	197.8	3.5E-07	3.8E+00	1.3E+03	0		3.5E-07	1.1E-07	3.5E-07				14%	-10.2	-10.9	-12.9
4-(2-naphthyl)-1,3-thiazol-2-amine	208-061-7	506-96-7	506967	665	Reach_1314	3694	123	-53.0	1.5E+04	3.2E+04	4.2E-01		0	4.5E-06	1.1E-06	3.5E-06				15%	-10.4	-10.9	-12.9
(1S)-2-(benzylamino)-1-[(2R)-6-fluoro-3,4-dihydro-2H-chromen	603-316-2	129050-27-7	129050277	1827	Reach_4116	3695	301	153.6	6.2E-07	4.9E+02	1.9E+03	13.8	5.76	1.1E-06	3.5E-08	1.1E-07				15%	-10.1	-10.9	-12.8
3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl acrylate	241-527-8	17527-29-6	17527296	2142	Reach_2436	3696	418	-7.6	2.9E+02	3.3E-01	5.9E+05			3.5E-06	3.5E-07	1.1E-06				20%	-11.2	-10.9	-14.2
retinyl propionate	806-749-7	918504-27-5	918504275	4022	Reach_5079	3697	458	261.2	2.0E-11	1.1E+00	1.6E+02			3.5E-07	3.5E-08	1.1E-07				23%	-10.8	-11.0	-12.0
4,4-Difluoro-N-[(1S)-3-hydroxy-1-phenylpropyl]cyclohexanecar	700-375-7	568572-17-8	568572178	3213	Reach_4880	3698	597	328.7	1.5E-17	4.3E-03	3.4E+06	8.01	0	3.5E-07	3.5E-08	1.1E-07				14%	-10.2	-11.0	-13.0
N,N'-[Methyl(vinyl)silanediyl]bis(N-ethylacetamide)	608-112-7	27566-05-8	27566058	2512	Reach_4260	3699	241	125.1	1.8E-04	1.8E+03	2.8E+03		6.27	1.1E-06	3.5E-08	1.1E-07				14%	-10.0	-11.0	-12.8
1,2-dibromo-3-chloropropane	700-662-7	950773-38-3	950773383	4119	Reach_4961	3700	481	205.6	3.6E-08	1.9E-05	2.2E+08			1.1E-06	1.1E-07	3.5E-07				23%	-11.3	-11.0	-12.8
611-200-8	700-160-8	82419-35-0	82419350	3824	Reach_4784	3701	281	167.4	3.2E-05	1.1E+02	8.7E+01	5.8		1.1E-06	1.1E-07	3.5E-07				14%	-10.3	-11.0	-12.9
678-409-4	805-125-1	1132940-51-2	1132940512	1616	Reach_5060	3702	416	106.1	4.2E-03	1.5E-01	2.1E+06			3.5E-07	1.1E-07	3.5E-07				23%	-10.7	-11.0	-12.0
heptadecafluorooctanesulphonyl fluoride	204-200-0	117-61-3	117613	1661	Reach_959	3703	344	277.2	4.3E-16	2.5E+03	6.6E-03			3.5E-06	1.1E-07	1.1E-06				22%	-10.9	-11.0	-13.5
(1R)-2-(benzylamino)-1-[(2S)-6-fluoro-3,4-dihydro-2H-chromen	600-381-9	1030385-16-0	1030385160	1356	Reach_4060	3704	301	153.6	6.2E-07	4.9E+02	1.9E+03	13.8	5.76	1.1E-06	3.5E-08	1.1E-07				15%	-10.1	-11.0	-12.9
14,14',15,15'-tetradehydro-7,7'-spirobi[dibenzo[b,g][1,9,4,6]di	695-716-9	1174931-74-8	1174931748	1658	Reach_4694	3705	449	216.5	2.1E-08	3.1E-01	5.2E+07			1.1E-06	1.1E-07	3.5E-07				21%	-10.3	-11.0	-12.4
3-ethyl-4-methyl-1,5-dihydro-2H-pyrrol-2-one	246-857-6	25333-42-0	25333420	2431	Reach_2566	3706	127	24.3	4.4E-02	7.6E+05	1.5E+00	15	3.8	3.5E-06	1.1E-07	1.1E-06				14%	-10.6	-11.0	-12.9
4-{6-[(methylsulfonyl)oxy]-1-benzothiophen-2-yl}phenyl metha	806-588-2	84449-65-0	84449650	3866	Reach_5076	3707	398	246.7	1.9E-10	3.2E+00	2.9E+03			1.1E-06	3.5E-08	1.1E-07				15%	-10.1	-11.0	-12.9
5-(methoxymethyl)-2-furaldehyde	700-445-7	846023-54-9	846023549	3870	Reach_4901	3708	309	168.9	2.5E-05	2.3E+03	1.7E+01			1.1E-06	1.1E-07	3.5E-07				14%	-11.2	-11.0	-12.9
5'-chloro-3-hydroxy-2'-methyl-2-naphthanilide	205-207-1	135-63-7	135637	1895	Reach_1134	3709	312	219.4	1.6E-09	1.0E+00	1.3E+05	10.2		1.1E-06	1.1E-07	3.5E-07				18%	-10.3	-11.0	-12.7
diphenhydramine	611-910-8	59886-90-7	59886907	3294	Reach_4368	3710	158	72.3	3.5E-01	6.8E+02	2.5E+00		13.7	3.5E-07	3.5E-08	1.1E-07				15%	-10.4	-11.0	-12.9
4-isothiocyanato-2-(trifluoromethyl)benzonitrile	700-185-4	1122460-01-8	1122460018	1579	Reach_4797	3711	255	134.2	2.9E-04	6.4E+01	7.2E+02			3.5E-06	3.5E-07	1.1E-06				18%	-11.3	-11.0	-12.4
2-amino-3,5-dibromobenzaldehyde	606-376-8	197721-70-3	197721703	2242	Reach_4208	3712	385	210.2	3.9E-10	1.4E+03	1.0E+03		0	1.1E-06	1.1E-07	3.5E-07				14%	-11.2	-11.0	-12.9
Dimethyl(octyl)amine oxide	607-854-9	2605-78-9	2605789	2451	Reach_4249	3713	173	137.3	2.5E-04	2.8E+01	5.1E+02		9.2	1.1E-06	1.1E-07	3.5E-07				14%	-10.4	-11.0	-13.0
2-(methoxymethyl)benzene-1,4-diamine	679-526-3	337906-36-2	337906362	2686	Reach_4621	3714	152	83.8	6.4E-02	6.4E+03	2.5E-01		7.72	1.1E-06	3.5E-07	1.1E-06				14%	-10.2	-11.0	-13.0
Ethyl (2S)-2-[(4S)-4-methyl-2,5-dioxo-1,3-oxazolidin-3-yl]penta	616-020-3	7381-13-7	7381137	3627	Reach_4421	3715	356	270.9	4.4E-12	5.3E+00	3.2E+02			1.1E-06	1.1E-07	3.5E-07				14%	-10.4	-11.0	-12.9
methyl 2-{[(4-hydroxyphenyl)sulfonyl]oxy}benzoate	700-604-0	947701-81-7	947701817	4114	Reach_4950	3716	402	206.3	2.0E-08	1.5E-03	1.9E+08	0		1.1E-06	1.1E-07	3.5E-07				15%	-10.2	-11.0	-12.9
ambroxol	609-132-9	35480-52-5	35480525	2739	Reach_4291	3717	318	106.9	1.3E-02	1.3E+01	3.2E+03	2.65	0	3.5E-06	1.1E-07	3.5E-07				14%	-10.2	-11.0	-12.9
metenolone	700-250-7	849793-87-9	849793879	3882	Reach_4821	3718	270	142.5	2.8E-04	7.0E+02	8.3E+01	4.37		3.5E-06	3.5E-07	1.1E-06				17%	-10.4	-11.0	-12.8
3-[(3-sulfanylbutanoyl)oxy]-2,2-bis{[(3-sulfanylbutanoyl)oxy]m	610-201-0	446292-08-6	446292086	2930	Reach_4327	3719	421	314.7	3.9E-15	4.5E+02	1.0E+02	0		1.1E-06	1.1E-07	3.5E-07				16%	-10.3	-11.0	-12.8
(4Z)-hept-4-en-2-yl salicylate	700-488-1	873888-84-7	873888847	3929	Reach_4910	3720	234	100.2	1.9E-03	6.7E-01	1.8E+05	9.8		1.1E-06	1.1E-07	3.5E-07				18%	-11.2	-11.0	-12.7
1-Bromomethyl-4-iodo-benzene	618-883-1	92878-95-0	92878950	4052	Reach_4502	3721	246	115.0	3.2E-03	1.2E+02	4.9E+02			1.1E-06	1.1E-07	3.5E-07				18%	-11.3	-11.0	-12.5
3-hydroxy-4-[(2-methyl-5-nitrophenyl)azo]-N-phenylnaphthale	229-245-3	6448-95-9	6448959	3436	Reach_2188	3722	426	290.0	1.2E-14	2.3E-02	1.7E+08	9.37		3.5E-07	1.1E-08	3.5E-08				23%	-10.9	-11.0	-11.8
(phenylethyl)benzene	801-277-8	507448-65-9	507448659	3018	Reach_5055	3723	197	-18.1	1.7E+02	2.5E+04	1.3E+01			3.5E-06	3.5E-07	1.1E-06				16%	-11.3	-11.1	-12.6
2-(4-fluorophenyl)thiophene	614-164-1	67911-21-1	67911211	3503	Reach_4396	3724	140	-4.1	6.8E+01	3.2E+04	8.1E+01			3.5E-06	3.5E-07	1.1E-06				15%	-11.3	-11.1	-12.5
(2S)-5-amino-2-[(aminoacetyl)amino]-5-oxopentanoic acid	229-929-1	6843-66-9	6843669	3516	Reach_2207	3725	244	75.0	3.9E-02	7.8E+00	1.0E+03	0	0	1.1E-06	1.1E-07	3.5E-07				14%	-9.7	-11.1	-13.1
(4S)-4-cyclohexyl-L-proline	619-510-5	141573-95-7	141573957	1937	Reach_4525	3726	204	52.0	3.5E+00	1.2E+03	1.9E+01	0	15.5	3.5E-06	3.5E-07	1.1E-06				14%	-10.0	-11.1	-13.0
pentyl 6-deoxy-alpha-L-mannopyranoside	800-300-9	83447-96-5	83447965	3847	Reach_5041	3727	364	35.0	3.7E-01	2.7E+00	3.4E+05	0		3.5E-07	1.1E-07	3.5E-07				14%	-10.1	-11.1	-13.0

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
dimethoxydiphenylsilane	202-662-8	98-37-3	98373	4183	Reach_505	3728	189	160.8	1.1E-06	1.3E+05	2.8E-03			3.5E-06	1.1E-07	3.5E-07				15%	-11.3	-11.1	-12.7
614-164-1	615-149-2	707-36-8	707368	3568	Reach_4411	3729	199	32.4	2.1E+01	4.8E+00	1.1E+05			3.5E-07	3.5E-08	1.1E-07				14%	-11.3	-11.1	-12.9
2-({[4-(3-methoxypropoxy)-3-methyl-1-oxidopyridin-2-yl]meth	642-214-2	924663-38-7	924663387	4035	Reach_4609	3730	375	285.3	4.4E-16	6.4E+00	6.0E+00	8.8	11	1.1E-06	1.1E-07	3.5E-07				14%	-10.0	-11.1	-13.1
611-382-9	611-382-9	5637-42-3	5637423	3193	Reach_4358	3731	160	113.8	6.4E-03	2.8E+03	5.4E+00		3.2	3.5E-06	3.5E-07	1.1E-06				14%	-10.4	-11.1	-13.1
cyclohexanecarbonitrile	225-200-7	4711-68-6	4711686	2963	Reach_2058	3732	307	221.7	1.1E-09	2.5E+00	1.1E+05			3.5E-07	3.5E-08	1.1E-07				16%	-11.4	-11.1	-12.4
3-aminopropane-1-sulphonic acid	222-977-4	3687-18-1	3687181	2780	Reach_1980	3733	139	80.5	6.9E-03	1.2E+05	1.3E-03	0.69	3.94	3.5E-06	1.1E-06	3.5E-06				14%	-9.9	-11.1	-13.0
2-(octyloxy)benzoic acid	608-139-4	27830-12-2	27830122	2519	Reach_4262	3734	250	130.3	4.2E-04	4.4E+00	1.1E+05	3.8		1.1E-06	3.5E-07	1.1E-06				14%	-10.5	-11.1	-13.0
17β-hydroxy-1α-methyl-5-αandrostan-3-one acetate	683-287-0	877670-90-1	877670901	3942	Reach_4628	3735	355	243.0	3.5E-10	2.7E+01	2.5E+02			1.1E-06	1.1E-07	3.5E-07				18%	-11.1	-11.1	-12.8
methylidynetri-p-phenylene triisocyanate	687-797-4	23551-91-9	23551919	5786	Reach_4640	3736	238	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				21%	-10.6	-11.1	-12.1
1,3-bis[(2-hydroxyethyl)thio]propan-2-ol	230-363-2	7069-42-3	7069423	3567	Reach_2222	3737	343	124.0	1.0E-04	6.6E-04	1.3E+09	0		3.5E-06	3.5E-07	1.1E-06				14%	-10.1	-11.1	-13.1
16α,17,21-trihydroxypregna-1,4,9(11)-triene-3,20-dione 21-ace	278-593-2	77017-20-0	77017200	3729	Reach_2949	3738	400	219.8	2.1E-11	2.7E+01	1.8E+03	12.4		1.1E-06	3.5E-07	1.1E-06				15%	-10.3	-11.1	-12.9
(3S)-3-hydroxy-4,4-dimethyldihydrofuran-2(3H)-one	626-470-2	5405-40-3	5405403	3120	Reach_4580	3739	130	31.2	5.5E-02	1.8E+05	1.1E-01	12.6		3.5E-06	3.5E-07	1.1E-06				14%	-10.1	-11.1	-13.3
5-methylnicotinic acid	608-720-2	3222-49-9	3222499	2645	Reach_4280	3740	137	76.5	3.3E-01	3.9E+03	1.7E+01	1.96	9.16	1.1E-06	1.1E-07	3.5E-07				14%	-10.2	-11.1	-13.1
2,6-dimethylphenyl 4-hydroxybenzenesulfonate	700-890-7	503614-91-3	503614913	3002	Reach_5019	3741	489	303.0	2.6E-14	2.0E+00	4.4E+03	0		3.5E-07	1.1E-07	3.5E-07				15%	-10.4	-11.1	-13.0
methyl 3-aminopyrazinecarboxylate	805-675-2	102340-61-4	102340614	1340	Reach_5069	3742	395	155.8	2.6E-06	9.9E-04	1.9E+09		0	1.1E-06	1.1E-07	3.5E-07				14%	-10.4	-11.1	-13.1
methyl 3-amino-5,6-dichloropyrazine-2-carboxylate	600-406-3	103201-78-1	103201781	1360	Reach_4062	3743	197	304.8	6.3E-09	4.6E+02	3.5E+00		3.4	1.1E-06	3.5E-07	1.1E-06				14%	-10.5	-11.1	-13.0
1,3-dihydro-1-oxoisobenzofuran-5-carbonitrile	700-420-0	7605-52-9	7605529	3696	Reach_4895	3744	156	-18.5	6.5E+01	3.0E+02	1.1E+03			1.1E-06	3.5E-07	1.1E-06				14%	-10.5	-11.1	-13.2
2,4-dihydro-5-methyl-3H-pyrazol-3-one	203-565-3	108-26-9	108269	1480	Reach_738	3745	98	99.7	1.3E-03	8.6E+04	1.7E+00		11.5	3.5E-06	1.1E-06	3.5E-06				14%	-10.2	-11.1	-13.0
15-tert-butyl 14a-ethyl (2R,6S,12Z,13aS,14aR,16aS)-6-{[(5-met	700-127-8	21862-63-5	21862635	536	Reach_4771	3746	156	4.3	1.4E+00	8.1E+01	2.6E+03	16	0	2.6E-07	1.1E-07	3.5E-07				15%	-10.4	-11.1	-13.0
10-hydroxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl) deca	700-609-8	1231148-36-9	1231148369	1762	Reach_4952	3747	517	291.4	1.7E-13	7.0E-04	8.5E+05	0		3.5E-07	3.5E-08	1.1E-07				16%	-10.3	-11.1	-12.9
2-Ethylhexyl-2-cyano-3-(4-methoxyphenyl)-3-phenylprop-2-en	700-213-5	947753-66-4	947753664	4115	Reach_4806	3748	392	199.3	6.5E-08	2.5E-02	9.1E+06			1.1E-06	1.1E-07	3.5E-07				21%	-10.7	-11.1	-12.3
ethyl (1R,2S)-1-{[(4R)-4-(phenanthridin-6-yloxy)-L-prolyl]amino	940-793-9	1432505-97-9	1432505979	1961	Reach_5174	3749	306	184.1	3.8E-07	4.3E+02	4.4E+02	7.95	0	1.1E-06	1.1E-07	3.5E-07				16%	-10.4	-11.1	-12.9
606-247-6	601-489-9	1176-81-4	1176814	1662	Reach_4091	3750	421	207.0	6.9E-10	3.6E+00	2.8E+02	15.6		1.1E-06	3.5E-07	1.1E-06				14%	-10.6	-11.1	-13.1
4,4-Difluoro-N-[(1S)-3-oxo-1-phenylpropyl]cyclohexanecarboxa	700-320-7	18916-17-1	18916171	2215	Reach_4859	3751	583	349.8	3.7E-25	6.5E+02	2.3E+00	9.03	0	1.1E-06	1.1E-07	3.5E-07				14%	-10.4	-11.1	-13.1
627-054-3	627-054-3	82410-32-0	82410320	3823	Reach_4582	3752	255	265.8	6.0E-15	5.3E+04	5.4E-02	9.37	11.9	1.1E-06	3.5E-07	1.1E-06				14%	-9.9	-11.1	-13.1
Methyl 5-amino-4-cyano-3-methylthiophene-2-carboxylate	700-422-1	61320-65-8	61320658	3331	Reach_4896	3753	196	125.1	2.7E-03	1.3E+03	2.4E+01			1.1E-06	1.1E-07	3.5E-07				14%	-10.5	-11.2	-13.2
616-651-4	700-301-3	69739-16-8	69739168	3549	Reach_4851	3754	585	349.8	1.1E-20	3.1E+00	5.1E+01			1.1E-07	3.5E-08	1.1E-07				23%	-11.1	-11.2	-11.8
2-[3-hydroxy-4-(phenylcarbonyl)phenoxy]ethyl 2-methylprop-2	700-105-8	16613-04-0	16613040	2102	Reach_4765	3755	326	177.6	4.2E-07	6.2E-01	2.9E+04	9.68		1.1E-06	1.1E-07	3.5E-07				16%	-10.5	-11.2	-13.0
3-amino-4-chlorobenzamide	243-231-4	19694-10-1	19694101	2236	Reach_2482	3756	171	135.9	8.1E-04	6.6E+03	3.0E+00	14.8	12.5	1.1E-06	3.5E-07	1.1E-06				14%	-10.2	-11.2	-13.1
604-269-0	303-725-3	94213-23-7	94213237	4099	Reach_3009	3757	256	155.3	3.7E-05	2.7E+01	2.3E+02		8.51	1.1E-07	1.1E-08	3.5E-08				14%	-11.4	-11.2	-12.9
tetraammonium ethylenediaminetetraacetate	245-022-3	22473-78-5	22473785	1206	Reach_2523	3758	360	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-10.9	-11.2	-12.8
610-915-2	630-348-4	84268-36-0	84268360	3858	Reach_4598	3759	339	224.5	6.9E-10	2.4E+01	2.0E+03		15.1	1.1E-06	1.1E-07	3.5E-07				14%	-11.4	-11.2	-12.9
2-[4-(Phenylmethoxy)phenyl]ethyldecanoate	700-058-3	848484-93-5	848484935	3877	Reach_4744	3760	383	179.3	9.3E-07	6.5E-04	1.9E+08			1.1E-06	1.1E-07	3.5E-07				23%	-10.8	-11.2	-12.0
pent-4-enoyl chloride	444-370-5	669005-94-1	669005941	3483	Reach_3737	3761	501	260.6	2.2E-11	2.1E-05	2.6E+09			1.1E-06	3.5E-07	1.1E-06				14%	-11.5	-11.2	-13.2
601-596-0	700-336-4	1141-23-7	1141237	1624	Reach_4866	3762	242	178.5	6.2E-06	1.7E+04	2.2E+01	4.38	14.8	1.1E-06	1.1E-07	3.5E-07				15%	-10.4	-11.2	-13.0
2-(methylsulfonyl)-3-nitropyrazolo[1,5-a]pyridine	223-768-0	4062-46-8	4062468	2861	Reach_2008	3763	347	149.8	4.7E-05	2.4E+00	3.1E+04			3.5E-07	3.5E-08	1.1E-07				14%	-10.2	-11.2	-13.3
4'-chloro-3-hydroxy-2',5'-dimethoxy-2-naphthanilide	224-270-6	4273-92-1	4273921	2898	Reach_2025	3764	358	236.1	1.0E-10	1.0E-01	5.2E+04	10.2		1.1E-06	3.5E-08	1.1E-07				17%	-10.4	-11.2	-13.0
(2R)-6-fluoro-2-[(2S)-oxiran-2-yl]chromane	603-315-7	129050-26-6	129050266	1826	Reach_4115	3765	194	58.3	1.0E+00	7.7E+02	4.7E+02			1.1E-06	3.5E-08	1.1E-07				15%	-11.4	-11.2	-13.0
(6-hydroxy-2-naphthyl)boronic acid	687-349-8	173194-95-1	173194951	2131	Reach_4633	3766	188	158.0	7.1E-08	0.0E+00	1.6E+02	8.86		1.1E-06	1.1E-07	3.5E-07				15%	-10.3	-11.2	-13.1
(17β)-17-hydroxyestra-4,6-dien-3-one	268-028-8	67990-05-0	67990050	3504	Reach_2895	3767	581	349.8	4.9E-21	2.7E-04	1.7E+08	9.39		3.5E-07	1.1E-08	3.5E-08				15%	-10.5	-11.2	-13.1
617-838-3	606-946-6	221640-14-8	221640148	5780	Reach_4228	3768	444	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				14%	-9.9	-11.2	-13.3
619-739-0	700-318-6	879671-67-7	879671677	6073	Reach_4858	3769	216	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-11.5	-11.2	-13.0
benzyl (5-{[4-({5-[acetyl(hydroxy)amino]pentyl}amino)-4-oxobu	218-378-2	2137-18-0	2137180	2292	Reach_1762	3770	316	170.3	2.2E-07	9.3E+01	4.3E+02	13.9	0	3.5E-07	3.5E-08	1.1E-07				14%	-10.1	-11.2	-13.3
(1E)-1-chloro-3,3,3-trifluoroprop-1-ene	700-486-0	102687-65-0	102687650	1351	Reach_4909	3771	131	-110.6	1.1E+05	4.3E+03	2.8E+02			3.5E-07	3.5E-08	1.1E-07				22%	-11.6	-11.2	-14.0
603-467-4	603-467-4	13127-18-9	13127189	1848	Reach_4122	3772	749	349.8	1.8E-26	1.1E-01	1.9E+02	11.8	5.45	3.5E-06	3.5E-07	1.1E-06				14%	-11.3	-11.2	-13.2
2-[2-(dimethylamino)ethyl]-2,3-dihydro-1H-inden-1-one	700-600-9	3409-21-0	3409210	2691	Reach_4947	3773	203	85.3	4.0E-02	7.0E+03	1.7E+02		4.7	1.1E-06	1.1E-07	3.5E-07				15%	-10.9	-11.2	-13.2
(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl methanesulfonat	700-367-3	35130-97-3	35130973	2724	Reach_4876	3774	219	99.3	2.3E-02	9.9E+04	1.7E+00		5.2	1.1E-06	3.5E-07	1.1E-06				14%	-10.4	-11.2	-13.3
(2R)-6-fluoro-2-[(2R)-oxiran-2-yl]chromane	606-373-1	197706-50-6	197706506	2240	Reach_4206	3775	194	58.3	1.0E+00	7.7E+02	4.7E+02			1.1E-06	3.5E-08	1.1E-07				15%	-11.5	-11.2	-13.1
(2S)-6-fluoro-2-[(2S)-oxiran-2-yl]chromane	603-314-1	129050-23-3	129050233	1825	Reach_4114	3776	194	58.3	1.0E+00	7.7E+02	4.7E+02			1.1E-06	3.5E-08	1.1E-07				15%	-11.5	-11.2	-13.1
(1S)-2,3,4,6-tetra-O-acetyl-1,5-anhydro-1-[4-chloro-3-(4-ethox	930-010-9	461432-25-7	461432257	2947	Reach_5129	3777	577	254.5	4.7E-11	7.2E-02	4.6E+04			1.1E-06	1.1E-07	3.5E-07				17%	-10.5	-11.3	-13.0
(1S)-3-(methylamino)-1-(2-thienyl)propan-1-ol	696-192-4	935859-71-5	935859715	4074	Reach_4709	3778	242	164.0	5.2E-05	2.1E+03	1.4E+00	0	0	1.1E-06	1.1E-07	3.5E-07				14%	-10.3	-11.3	-13.3
(2R)-2,8-dimethyl-2-[(4R,8R)-4,8,12-trimethyltridecyl]-3,4-dihy	606-247-6	191605-10-4	191605104	2223	Reach_4200	3779	418	236.4	9.7E-10	1.8E+03	1.1E+04	1.1		1.1E-06	1.1E-07	3.5E-07				23%	-11.1	-11.3	-11.9
6-Chlorohexanoic acid	212-406-7	814-80-2	814802	6042	Reach_1551	3780	218	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-10.8	-11.3	-13.2
2-tert-butyl-4,6-diiodophenol	805-179-6	60803-26-1	60803261	3316	Reach_5063	3781	402	122.6	4.0E-04	7.5E+00	5.8E+05	7.8		3.5E-06	3.5E-07	1.1E-06				18%	-11.3	-11.3	-13.0
2-[(3-nitropyrazolo[1,5-a]pyridin-2-yl)oxy]ethanol	689-267-8	501925-98-0	501925980	2997	Reach_4650	3782	529	189.3	2.1E-07	6.5E+00	3.1E+00	11.3		1.1E-06	1.1E-07	1.1E-06				14%	-10.3	-11.3	-13.3
N-[(2-methyl-5-nitrophenyl)carbamothioyl]acetamide	607-485-3	25015-63-8	25015638	2413	Reach_4242	3783	128	-25.1	4.1E+03	0.0E+00	2.8E+00	0	0	1.1E-06	3.5E-07	1.1E-06				14%	-10.3	-11.3	-13.5
2-(2-Methoxyphenoxy)ethanamine	700-396-1	60924-38-1	60924381	3320	Reach_4886	3784	457	230.0	1.1E-11	6.9E+00	3.2E+02		0	1.1E-06	1.1E-07	3.5E-07				14%	-11.0	-11.3	-13.3
1,4,5,6-tetrahydro-1,2-dimethylpyrimidine	260-375-3	56773-42-3	56773423	5936	Reach_2822	3785	629	0.0	0.0E+00	0.0E+00	0.0E+00		0	0.0E+00	0.0E+00	0.0E+00				14%	-11.5	-11.3	-12.9
4-({4-[4-(4-{[4-(Propan-2-yloxy)phenyl]sulfonyl}phenoxy)butox	638-778-4	376348-77-5	376348775	2803	Reach_4602	3786	297	173.6	7.4E-08	1.4E+02	3.2E+02	13.8		1.1E-06	1.1E-07	3.5E-07				21%	-10.6	-11.3	-12.5
601-489-9	619-702-9	33494-80-3	33494803	5848	Reach_4538	3787	248	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				15%	-10.5	-11.3	-13.1
605-935-3	605-935-3	181525-38-2	181525382	2168	Reach_4184	3788	220	181.3	2.4E-08	6.8E+02	6.2E-01	15.9	12.3	3.5E-06	1.1E-06	3.5E-06				14%	-10.2	-11.3	-13.2
(2S)-6-fluoro-2-[(2R)-oxiran-2-yl]chromane	606-374-7	197706-51-7	197706517	2241	Reach_4207	3789	194	58.3	1.0E+00	7.7E+02	4.7E+02			1.1E-06	3.5E-08	1.1E-07				15%	-11.6	-11.3	-13.1
(2S)-pentan-2-ol	680-808-3	106261-64-7	106261647	5598	Reach_4627	3790	326	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-11.6	-11.3	-12.7
strontium 4-[(4-chloro-5-methyl-2-sulphonatophenyl)azo]-3-hy	267-291-6	67828-72-2	67828722	5988	Reach_2890	3791	506	0.0	0.0E+00	0.0E+00	0.0E+00									18%	-11.0	-11.3	-13.0
(5R)-5-[(1S)-1,2-Dihydroxyethyl]-4-ethoxy-3-hydroxyfuran-2(5H	617-849-3	86404-04-8	86404048	3906	Reach_4477	3792	204	143.9	1.5E-07	4.4E+05	4.9E-04	13.5		3.5E-06	3.5E-07	1.1E-06				14%	-10.2	-11.3	-13.6
phenethylamine	700-928-2	143782-23-4	143782234	1970	Reach_5028	3793	228	84.8	7.8E-02	9.3E+00	2.5E+04		0	3.5E-07	3.5E-08	1.1E-07				16%	-11.6	-11.3	-12.7
(3aS,4R,5S,6S,8R,9R,9aR,10R)-6-ethenyl-5-hydroxy-4,6,9,10-tet	700-114-7	143183-03-3	143183033	1958	Reach_4768	3794	579	335.8	1.3E-16	7.4E-06	2.5E+09	0		3.5E-07	1.1E-08	3.5E-08				15%	-10.5	-11.3	-13.2
chloromethyl chlorosulphate	700-938-7	72716-26-8	72716268	6012	Reach_5031	3795	396	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				14%	-11.6	-11.3	-13.2
1-tert-butyl-3,5-diiodo-2-methoxybenzene	229-102-5	6410-32-8	6410328	3424	Reach_2178	3796	440	295.4	4.6E-15	7.8E-03	1.7E+08			3.5E-07	1.1E-08	3.5E-08				21%	-11.5	-11.3	-12.7
hexane-1,6-diyl bis{[3-(trimethoxysilyl)propyl]carbamate}	610-764-2	51997-51-4	51997514	3050	Reach_4335	3797	239	152.6	4.5E-05	8.0E+00	7.1E+02	0		1.1E-06	3.5E-08	1.1E-07				14%	-10.5	-11.3	-13.4
undec-10-en-1-yl 2-cyano-3,3-diphenylacrylate	806-439-1	1364731-90-7	1364731907	1900	Reach_5072	3798	278	173.9	1.7E-06	1.7E+01	3.5E+03			1.1E-06	1.1E-07	3.5E-07				23%	-10.9	-11.4	-12.1
bis(nonafluorobutyl)phosphinic acid	248-660-0	27794-93-0	27794930	5812	Reach_2612	3799	528	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				22%	-11.8	-11.4	-13.4
700-627-6	610-150-4	438193-30-7	438193307	5887	Reach_4324	3800	526	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				23%	-11.5	-11.4	-12.5
2-(octyloxy)benzoyl chloride	250-799-7	31775-20-9	31775209	2632	Reach_2656	3801	718	349.8	1.3E-21	1.3E-05	1.6E+08			3.5E-07	3.5E-08	3.5E-08				17%	-11.6	-11.4	-12.9
Propane-1,3-diyl dioctanoate	700-787-7	769953-18-6	769953186	6034	Reach_4994	3802	288	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				21%	-11.5	-11.4	-12.8

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Tripropan-2-ylsilyl 2-methylprop-2-enoate	700-182-8	134652-60-1	134652601	1880	Reach_4795	3803	242	-14.5	1.3E+01	0.0E+00	6.0E+05			3.5E-06	3.5E-07	1.1E-06				20%	-11.6	-11.4	-14.6
trans-4-tert-butylcyclohexanol	202-667-5	98-42-0	98420	4184	Reach_506	3804	203	142.5	3.9E-06	5.2E+04	1.0E-02	-0.2		1.1E-06	1.1E-07	1.1E-06				17%	-11.7	-11.4	-12.7
2,2-dimethoxy-1,2-diphenylethan-1-one	680-046-1	74462-02-5	74462025	3637	Reach_4623	3805	298	162.5	6.5E-07	4.4E-01	1.1E+06			1.1E-06	3.5E-08	1.1E-07				15%	-11.5	-11.4	-13.3
7,7,8,9,9-pentamethyl-6,7,8,9-tetrahydro-5H-cyclopenta[h]quin	801-093-8	1315251-11-6	1315251116	1849	Reach_5052	3806	242	116.7	8.8E-03	1.0E+01	4.4E+04		10.5	1.1E-07	3.5E-08	1.1E-07				19%	-11.0	-11.4	-13.0
4-(Oxiran-2-ylmethoxy)-9H-carbazole	601-680-7	120202-68-8	120202688	5625	Reach_4100	3807	554	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				15%	-11.0	-11.4	-13.4
Tert-butyl 3-oxoazetidine-1-carboxylate	605-390-1	165115-73-1	165115731	2095	Reach_4173	3808	228	85.9	4.6E-04	2.8E+02	5.2E+02		0	1.1E-06	1.1E-07	3.5E-07				14%	-10.7	-11.4	-13.3
(chloromethyl)(methoxy)dimethylsilane	300-199-7	93924-07-3	93924073	4092	Reach_3004	3809	170	-20.9	3.1E+01	3.5E-02	1.7E+06			3.5E-07	3.5E-08	1.1E-07				19%	-11.7	-11.4	-13.5
617-556-0	609-734-1	39648-67-4	39648674	2845	Reach_4310	3810	348	90.3	2.4E-08	4.4E-05	1.7E+05	1.5		1.1E-07	3.5E-09	1.1E-08				14%	-10.4	-11.4	-13.4
2-({1-[(2-methoxyphenyl)amino]-1,3-dioxobutan-2-yl}diazenyl)	691-722-0	154477-55-1	154477551	2036	Reach_4670	3811	514	262.8	2.8E-14	5.0E-02	2.8E+06	13.4	4.95	1.1E-06	1.1E-07	3.5E-07				15%	-10.5	-11.4	-13.3
5-bromonicotinic acid	244-065-5	20826-04-4	20826044	2275	Reach_2500	3812	202	99.8	5.0E-02	1.7E+03	3.8E+01	3.43	13.3	1.1E-06	1.1E-07	3.5E-07				14%	-10.6	-11.4	-13.5
2-chloro-1,1,1-triethoxyethane	628-654-8	51076-95-0	51076950	3027	Reach_4587	3813	197	10.6	1.7E+01	5.6E+02	7.2E+02			3.5E-07	1.1E-07	3.5E-07				16%	-11.7	-11.4	-12.8
(1R,2S,5R)-5-methyl-2-(propan-2-yl)cyclohexyl (ethylamino)(ox	209-502-6	583-39-1	583391	3244	Reach_1382	3814	150	118.9	4.8E-06	1.1E+03	8.5E+01	11.6		1.1E-06	1.1E-07	3.5E-07				14%	-11.1	-11.4	-13.3
(2R)-2-methyloxirane	800-036-4	1422423-64-0	1422423640	5694	Reach_5035	3815	384	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				17%	-11.8	-11.4	-13.4
4-[(4-oxo-1,4-dihydropyrimidin-2- yl)amino]benzonitrile	606-195-4	189956-45-4	189956454	2220	Reach_4197	3816	212	204.3	1.3E-07	1.2E+03	3.5E+00	9.29	8.85	3.5E-06	1.1E-06	3.5E-06				14%	-10.5	-11.4	-13.3
hexanoic anhydride	687-786-4	1246610-75-2	1246610752	5638	Reach_4638	3817	376	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				20%	-11.7	-11.4	-13.6
phentermine	200-991-1	76-89-1	76891	3726	Reach_178	3818	242	110.2	1.7E-04	5.1E+02	1.6E+02		0	1.1E-06	1.1E-07	3.5E-07				20%	-11.8	-11.4	-13.6
2-(Diethylamino)ethyl 4-{[2-(octyloxy)benzoyl]amino}benzoate	692-852-0	26090-29-9	26090299	2453	Reach_4681	3819	469	260.3	2.3E-11	1.0E-02	1.3E+07	14.3	5.2	1.1E-06	1.1E-07	3.5E-07				21%	-10.9	-11.4	-12.6
695-716-9	629-247-8	183208-35-7	183208357	2180	Reach_4590	3820	197	89.5	6.2E-02	9.6E+02	8.3E+01			3.5E-07	3.5E-08	1.1E-07				22%	-10.9	-11.4	-12.4
2-(methylthio)-3-nitropyrazolo[1,5-a]pyridine	619-167-1	95748-46-2	95748462	4132	Reach_4511	3821	495	331.7	1.1E-20	2.6E+02	5.5E+00			1.1E-06	1.1E-07	3.5E-07				15%	-11.1	-11.5	-13.4
5,7-di-tert-butyl-3-[4-(2-hydroxyethoxy)phenyl]-1-benzofuran-2	940-050-9	1216942-04-9	1216942049	1734	Reach_5164	3822	791	349.8	1.8E-24	7.5E-06	3.5E+07	12.4		1.1E-06	1.1E-07	3.5E-07				19%	-10.8	-11.5	-13.1
2-chloro-6,7-dimethoxyquinazolin-4-amine	245-821-7	23680-84-4	23680844	2354	Reach_2532	3823	240	153.0	2.0E-04	7.7E+02	3.2E+01		14.2	1.1E-06	1.1E-07	3.5E-07				14%	-10.6	-11.5	-13.5
2-[2-(2,4-difluorophenyl)prop-2-en-1-yl]propane-1,3-diol	690-742-7	1266664-66-7	1266664667	5645	Reach_4661	3824	302	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				15%	-10.9	-11.5	-13.4
5-tert-butyl-3-methyl-1,2-phenylene dibenzoate	691-553-2	1232839-86-9	1232839869	1766	Reach_4669	3825	388	163.6	1.4E-06	3.3E-02	1.7E+07			1.1E-06	1.1E-07	3.5E-07				21%	-11.0	-11.5	-12.6
9β,11β-epoxy-17,21-dihydroxy-16α-methylpregna-1,4-diene-3,	246-529-2	24916-90-3	24916903	2406	Reach_2556	3826	372	206.1	2.7E-10	6.7E+01	7.6E+01	13.2		1.1E-06	3.5E-07	1.1E-06				14%	-10.6	-11.5	-13.3
retinol	200-683-7	68-26-8	68268	3514	Reach_93	3827	286	111.2	3.1E-05	3.7E-01	4.2E+07	15.5		3.5E-06	3.5E-07	1.1E-06				21%	-11.1	-11.5	-12.7
629-671-3	213-214-6	930-33-6	930336	4057	Reach_1606	3828	85	111.2	5.7E-03	3.3E+05	3.0E-03	0		3.5E-06	1.1E-06	3.5E-06				14%	-11.7	-11.5	-13.2
4-butylbenzene-1,3-diol	700-906-2	22450-96-0	22450960	5783	Reach_5022	3829	469	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				15%	-11.3	-11.5	-13.4
pyridine-2,4-dicarboxylic acid	207-892-2	499-80-9	499809	2991	Reach_1298	3830	167	141.2	4.5E-05	8.1E+03	3.7E+00	0.32	8.72	3.5E-06	3.5E-07	1.1E-06				14%	-10.5	-11.5	-13.5
methyl trichloroacetate	209-960-7	598-99-2	598992	3295	Reach_1407	3831	177	-22.6	4.5E+02	2.4E+03	5.4E+01			1.1E-06	1.1E-07	3.5E-07				15%	-11.8	-11.5	-13.3
N-Palmitoylglycine	627-023-4	2441-41-0	2441410	2392	Reach_4581	3832	313	202.5	1.7E-07	4.1E-01	7.1E+05	3.5		1.1E-06	1.1E-07	3.5E-07				14%	-10.9	-11.5	-13.4
9-fluoro-11β,17,21-trihydroxy-16β-methylpregna-1,4-diene-3,2	609-203-4	36130-02-6	36130026	2757	Reach_4292	3833	461	223.9	3.3E-11	1.9E+00	5.1E+03	15.6		3.5E-06	3.5E-07	1.1E-06				15%	-10.7	-11.5	-13.3
(2Z,16Z)-4,15-dioxo-5,8,11,14-tetraoxaoctadeca-2,16-diene-1,1	806-734-5	109828-01-5	109828015	1509	Reach_5078	3834	346	187.1	3.5E-07	1.4E+04	2.4E+00	2.98		3.5E-06	3.5E-07	1.1E-06				14%	-10.4	-11.5	-13.5
4-[(2,4-dichloro-5-methoxyphenyl)amino]-6-methoxy-7-[3-(4-m	601-437-5	116539-55-0	116539550	1651	Reach_4089	3835	171	72.1	1.8E-02	6.4E+04	6.3E+00	15.4	3.47	1.1E-06	1.1E-07	3.5E-07				16%	-10.7	-11.5	-13.3
1,1,1-Trimethoxy-2-methylpropane	606-318-1	19478-81-0	19478810	5760	Reach_4204	3836	236	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				15%	-11.8	-11.5	-13.4
4,4-dimethyl-1,2-oxazolidin-3-one	629-718-8	127946-77-4	127946774	5651	Reach_4595	3837	119	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-11.1	-11.5	-13.6
6-hydroxy-3,4-dihydroquinolin-2(1H)-one	700-003-3	56519-71-2	56519712	3200	Reach_4721	3838	328	3.8	1.1E-02	2.5E-01	6.2E+06	0	0	1.1E-06	1.1E-07	3.5E-07				14%	-10.6	-11.5	-13.4
ethyl 2-cyano-3-oxobutanoate	602-769-3	122397-96-0	122397960	1749	Reach_4104	3839	328	218.9	7.9E-12	8.8E+03	1.9E-01	12.5		1.1E-06	1.1E-07	3.5E-07				14%	-11.7	-11.5	-13.6
Octadecyl 2-[(E)-(5-cyano-1-dodecyl-2-hydroxy-4-methyl-6-oxo	610-309-8	4651-94-9	4651949	2955	Reach_4328	3840	152	92.8	6.0E-02	7.1E+02	1.2E+02	0	0	3.5E-07	3.5E-08	1.1E-07				14%	-10.7	-11.6	-13.4
608-783-6	695-996-2	510729-01-8	510729018	3026	Reach_4701	3841	324	128.6	5.5E-04	3.5E+00	3.5E+04			1.1E-06	1.1E-07	3.5E-07				18%	-11.8	-11.6	-13.8
1-bromooctane	203-912-9	111-83-1	111831	312	Reach_874	3842	193	-17.9	6.9E+01	2.5E+00	4.1E+04			5.0E-07	1.1E-07	3.5E-07				22%	-11.9	-11.6	-14.3
propiolactone	200-340-1	57-57-8	57578	3233	Reach_42	3843	72	-52.8	3.1E+02	2.0E+05	1.6E-01			3.5E-06	3.5E-07	1.1E-06				14%	-11.8	-11.6	-13.5
1-Chloro-3,5-dimethyladamantane	616-314-1	76272-34-9	76272349	3707	Reach_4433	3844	230	125.1	2.5E-05	5.5E+02	1.7E+01			3.5E-07	3.5E-08	1.1E-07				22%	-11.9	-11.6	-14.0
16-({(1S)-1-carboxy-4-[(2,5-dioxopyrrolidin-1-yl)oxy]-4-oxobuty	700-853-5	943586-12-7	943586127	4102	Reach_5013	3845	513	349.8	7.4E-18	2.5E+00	9.3E+01	3.17		1.1E-06	1.1E-07	3.5E-07				14%	-10.7	-11.6	-13.6
1H-indazole-3-carboxylic acid	601-596-0	119302-24-8	119302248	1688	Reach_4095	3846	489	232.9	6.7E-12	1.5E+00	2.1E+03	14.9	5.31	1.1E-06	1.1E-07	3.5E-07				14%	-10.6	-11.6	-13.6
3-Methoxy-3-methylbutyl acetate	700-029-5	824-80-6	824806	6044	Reach_4450	3847	182	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				15%	-11.9	-11.6	-13.1
Ethyl 3-(difluoromethyl)-1-methyl-1H-pyrazole-4-carboxylate	804-748-6	1216941-97-7	1216941977	1732	Reach_5057	3848	291	204.5	1.3E-07	1.0E+01	2.0E+04		13.7	3.5E-06	3.5E-07	1.1E-06				14%	-10.8	-11.6	-13.6
Alkanes, C10-14	220-254-8	2688-84-8	2688848	2490	Reach_1854	3849	185	91.2	1.1E-01	5.6E+01	1.9E+02			1.1E-06	1.1E-07	3.5E-07				23%	-11.9	-11.6	-14.4
vinylene carbonate	212-825-5	872-36-6	872366	3923	Reach_1579	3850	86	13.9	4.7E-01	4.3E+04	2.8E-01			3.5E-06	3.5E-07	1.1E-06				14%	-11.0	-11.6	-13.7
2-methylquinolin-8-amine	606-190-7	18978-78-4	18978784	2218	Reach_4195	3851	158	94.5	2.6E-02	3.2E+02	3.7E+02		9.98	1.1E-06	3.5E-07	1.1E-06				14%	-11.0	-11.6	-13.5
1,5,2,4-dioxadithiane 2,2,4,4-tetraoxide	700-464-0	99591-74-9	99591749	4207	Reach_4903	3852	188	109.6	1.0E-02	3.3E+05	1.4E-01			1.1E-05	1.1E-06	3.5E-06				14%	-10.7	-11.6	-13.7
1,1,1,3,4,4,4-heptafluoro-3-(trifluoromethyl)butan-2-one	690-995-3	756-12-7	756127	3677	Reach_4663	3853	266	-71.2	3.2E+04	3.6E+01	6.6E+01			1.1E-06	3.5E-07	1.1E-06				20%	-11.9	-11.6	-14.6
2-methylresorcinol	213-313-4	936-49-2	936492	4076	Reach_1611	3854	146	109.0	4.5E-03	6.2E+04	2.8E+02	0		3.5E-07	3.5E-08	1.1E-07				14%	-10.9	-11.6	-13.5
2-chloro-5-nitrobenzoic acid	219-739-7	2516-96-3	2516963	2421	Reach_1826	3855	202	125.6	8.9E-04	5.2E+02	9.8E+01	2.16		1.1E-06	3.5E-08	1.1E-07				14%	-10.8	-11.7	-13.8
4,4'-(2-ethylhexane-1,1-diyl)diphenol	246-386-6	24650-42-8	24650428	2400	Reach_2552	3856	256	110.2	2.3E-03	7.3E+01	8.9E+02	0		1.1E-06	1.1E-07	3.5E-07				20%	-11.3	-11.7	-13.2
611-909-2	241-543-5	17572-97-3	17572973	5740	Reach_2437	3857	407	0.0	0.0E+00	0.0E+00	0.0E+00	0		0.0E+00	0.0E+00	0.0E+00				14%	-10.7	-11.7	-13.7
cyclopentadiene	692-842-6	1312296-85-7	1312296857	5660	Reach_4680	3858	250	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				20%	-12.0	-11.7	-14.5
4,4,5,5-Tetramethyl-1,3,2-dioxaborolane	691-441-3	1316184-79-8	1316184798	5662	Reach_4667	3859	776	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				14%	-12.0	-11.7	-13.2
deferoxamine	200-738-5	70-51-9	70519	3564	Reach_96	3860	561	349.8	8.4E-26	5.1E+04	2.9E-03	7.89	3.37	1.1E-06	1.1E-07	3.5E-07				14%	-10.6	-11.7	-13.9
(2S)-tetrahydrofuran-2-carboxylic acid	677-278-0	89402-42-6	89402426	3974	Reach_4617	3861	183	-18.6	3.3E+03	7.2E+02	1.5E+02	0		3.5E-07	3.5E-08	1.1E-07				14%	-10.6	-11.7	-13.7
2-(3,5-dimethylhex-3-en-2-yloxy)-2-methylpropyl cyclopropane	700-118-9	676532-44-8	676532448	3498	Reach_4769	3862	268	46.3	1.9E-01	6.7E+01	7.9E+04			3.5E-06	3.5E-07	1.1E-06				17%	-11.9	-11.7	-13.6
methyl 2-methyl-2-phenylpropanoate	617-556-0	84348-37-8	84348378	3861	Reach_4467	3863	229	131.7	1.2E-03	4.9E+04	3.1E+00			3.5E-06	3.5E-07	1.1E-06				15%	-12.0	-11.8	-13.2
(2S)-2-{[(5-methylpyrazin-2-yl)carbonyl]amino}non-8-enoic acid	700-643-3	155794-06-2	155794062	2044	Reach_4958	3864	383	209.1	1.9E-10	1.9E-01	3.7E+05	14.7	0	1.1E-06	1.1E-07	3.5E-07				16%	-11.0	-11.8	-13.6
methyl cis-3-methylcyclohexanecarboxylate	680-002-1	145022-44-2	145022442	5699	Reach_4622	3865	261	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				15%	-12.1	-11.8	-13.5
1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluorooctane	688-332-8	199119-58-9	199119589	5764	Reach_4644	3866	459	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				22%	-12.1	-11.8	-14.8
Octan-2-yl 2-cyanoacrylate	938-829-3	936103-10-5	936103105	4075	Reach_5154	3867	224	156.2	4.1E-06	3.8E+03	1.4E+01			1.1E-06	1.1E-07	3.5E-07				16%	-12.1	-11.8	-13.5
(Bromomethyl)cyclobutane	261-858-1	59690-88-9	59690889	5943	Reach_2840	3868	188	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				22%	-12.2	-11.9	-14.4
Ethyl [(5-chlorothiophen-2-yl)sulfonyl]carbamate	700-455-1	380843-75-4	380843754	2814	Reach_4902	3869	530	278.3	1.3E-12	2.2E-01	2.1E+04	14.7	5.95	1.1E-06	3.5E-08	1.1E-07				14%	-11.0	-11.9	-13.8
O,S-dibutyl dithioimidodicarbonate	691-061-8	1001320-38-2	1001320382	1294	Reach_4664	3870	249	101.8	5.8E-03	2.3E+01	5.0E+03	8.5		3.5E-06	3.5E-07	1.1E-06				15%	-12.2	-11.9	-13.8
methyl 2-[4-(4-{4-[hydroxy(diphenyl)methyl]piperidin-1-yl}buta	601-595-5	119302-20-4	119302204	1687	Reach_4094	3871	447	228.3	4.4E-12	3.0E+01	5.4E+02	14.7	4.21	3.5E-07	3.5E-08	1.1E-07				20%	-11.4	-11.9	-13.3
689-732-5	611-173-2	54605-02-6	54605026	3148	Reach_4350	3872	539	238.6	2.3E-12	2.0E-01	1.0E+04	14.1	0	3.5E-06	3.5E-07	1.1E-06				14%	-11.2	-12.0	-13.9
3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl 2-chloroacrylate	801-260-5	96383-55-0	96383550	4146	Reach_5054	3873	453	7.9	8.4E+01	9.3E-02	1.8E+06			3.5E-06	3.5E-07	1.1E-06				21%	-12.2	-12.0	-15.2
609-203-4	627-725-0	398489-26-4	398489264	2850	Reach_4585	3874	171	47.3	3.8E+00	1.7E+04	4.6E+01	0		1.1E-06	1.1E-07	1.1E-06				15%	-11.2	-12.0	-13.9
800-300-9	692-895-5	81778-07-6	81778076	3813	Reach_4682	3875	115	72.0	6.9E-01	6.0E+04	2.0E+00			3.5E-06	3.5E-07	1.1E-06				20%	-12.3	-12.0	-13.7
(2Z)-1,1,1,4,4,4-Hexafluorobut-2-ene	700-651-7	692-49-9	692499	3536	Reach_4960	3876	164	-127.4	3.3E+05	3.4E+01	8.3E+02			1.1E-06	1.1E-07	3.5E-07				20%	-12.4	-12.1	-15.1
611-173-2	606-191-2	18979-61-8	18979618	2219	Reach_4196	3877	166	89.4	9.8E-03	9.4E+02	1.1E+03	9.6		1.1E-06	1.1E-07	3.5E-07				15%	-11.2	-12.1	-13.9

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
bromoethylene	606-080-9	18637-00-8	18637008	5749	Reach_4192	3878	201	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				22%	-12.5	-12.1	-14.8
2-({[3-(methylthio)phenyl]carbamoyl}oxy)ethyl acrylate	700-694-1	1207339-61-4	1207339614	1719	Reach_4970	3879	281	50.8	6.8E-03	1.5E+02	5.5E+02	12.7		1.1E-06	1.1E-07	3.5E-07				15%	-12.3	-12.2	-14.1
acetyl bromide	606-740-6	21331-43-1	21331431	2290	Reach_4216	3880	226	162.0	2.6E-05	5.2E+00	5.9E+03			1.1E-06	1.1E-07	3.5E-07				14%	-12.5	-12.2	-14.4
2-methyl-2-(1-methylpropyl)propane-1,3-diol	212-387-5	813-60-5	813605	3805	Reach_1550	3881	146	21.5	4.8E-01	6.1E+03	3.6E+01	15.3		1.1E-06	3.5E-07	1.1E-06				14%	-12.4	-12.2	-14.1
methyl cyclohexylacetate	805-128-8	54981-42-9	54981429	5928	Reach_5062	3882	329	0.0	0.0E+00	0.0E+00	0.0E+00			0.0E+00	0.0E+00	0.0E+00				17%	-12.5	-12.3	-13.8
2,3-difluoro-5-(trifluoromethyl)pyridine	627-872-0	1514-82-5	1514825	2019	Reach_4586	3883	175	-92.6	3.9E+04	1.9E+03	3.1E+02			3.5E-07	3.5E-08	1.1E-07				21%	-12.6	-12.3	-14.8
607-821-9	607-821-9	25858-24-6	25858246	2445	Reach_4248	3884	354	213.3	3.3E-08	2.1E+00	9.8E+03			1.1E-06	1.1E-07	3.5E-07				16%	-11.5	-12.3	-14.1
2,3,3,3-tetrafluoro-2-(trifluoromethyl)propanenitrile	806-451-7	42532-60-5	42532605	2895	Reach_5073	3885	195	-69.1	2.2E+04	7.6E+00	1.6E+02			3.5E-07	1.1E-07	3.5E-07				22%	-12.6	-12.3	-15.1
(1R,2S,5R)-5-methyl-2-(propan-2-yl)-N-[2-(pyridin-2-yl)ethyl]cy	700-097-6	847565-09-7	847565097	3876	Reach_4760	3886	288	173.2	5.8E-06	3.0E+02	2.1E+04	14.3	8.33	1.1E-06	1.1E-07	3.5E-07				15%	-11.6	-12.3	-14.1
2-bromo-3,3,3-trifluoroprop-1-ene	618-003-6	87392-07-2	87392072	3930	Reach_4484	3887	116	33.5	1.8E+01	5.2E+04	1.3E+00			3.5E-06	3.5E-07	1.1E-06				22%	-12.7	-12.3	-15.1
Methyl 2,2,3,3,4,4-hexafluoro-4-[(trifluorovinyl)oxy]butanoate	700-713-3	83161-22-2	83161222	3841	Reach_4976	3888	234	121.4	5.0E-06	7.3E+03	6.5E+00			1.1E-06	3.5E-07	1.1E-06				18%	-12.7	-12.4	-15.6
2,5-Bis-O-{4-[4-(acryloyloxy)benzoyl]-3-methoxybenzoyl}-1,4:3,	700-376-2	1015689-48-1	1015689481	1324	Reach_4881	3889	795	349.8	7.1E-19	1.0E-04	1.2E+04			1.1E-06	1.1E-07	3.5E-07				16%	-11.8	-12.5	-14.3
Methyl butylcarbamate	805-660-0	2594-21-0	2594210	2447	Reach_5068	3890	131	-18.4	2.4E+02	1.2E+04	2.7E+01	12		3.5E-06	1.1E-07	3.5E-07				14%	-12.8	-12.6	-14.3
2,2,3,3-Tetrafluorooxetane	700-202-5	765-63-9	765639	3718	Reach_4801	3891	130	-85.8	1.8E+05	1.6E+04	8.9E+01			1.1E-06	1.1E-07	3.5E-07				19%	-13.2	-12.8	-15.5
ethyl cyclopent-2-en-1-ylacetate	605-150-6	15848-49-4	15848494	2062	Reach_4168	3892	154	-12.3	4.7E+01	2.0E+03	8.3E+02			3.5E-06	3.5E-07	1.1E-06				14%	-13.3	-13.1	-14.7
3-[(4R)-4-Isopropylcyclohex-1-en-1-yl]propanal	700-886-5	1378867-81-2	1378867812	1914	Reach_5018	3893	180	16.1	3.5E+00	3.0E+01	2.1E+04			3.5E-07	1.1E-07	3.5E-07				18%	-13.5	-13.2	-14.7
3-(cyclohexyloxy)propane-1,2-diol	805-622-3	10305-41-6	10305416	1358	Reach_5067	3894	174	56.0	7.9E-03	9.6E+04	1.3E+01	14.1		3.5E-06	1.1E-06	3.5E-06				14%	-13.2	-14.0	-15.9
octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	218-216-0	2082-79-3	2082793	2276	Reach_1755	3895	531	241.0	4.5E-11	5.0E-08	2.6E+13	11.9		1.1E-06	1.1E-07	3.5E-07							
2,6,10,15,19,23-hexamethyltetracosane	203-825-6	111-01-3	111013	1535	Reach_841	3896	423	74.7	3.7E-02	6.7E-09	4.3E+14			1.1E-06	1.1E-07	3.5E-07							
1,3,5-tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6	248-597-9	27676-62-6	27676626	2516	Reach_2611	3897	784	349.8	6.2E-26	3.3E-10	1.5E+15	10.7	13	1.1E-06	1.1E-07	3.5E-07							
5,5'-(1H-isoindole-1,3(2H)-diylidene)dibarbituric acid	253-256-2	36888-99-0	36888990	2783	Reach_2706	3898	367	349.8	7.5E-23	1.2E+04	1.2E-02	1.7	-0.76	1.1E-06	3.5E-08	1.1E-07				14%			
607-578-9	203-727-3	110-00-9	110009	270	Reach_799	3899	68	-87.1	7.9E+04	8.1E+03	2.3E+01			2.2E-09	1.1E-07	3.5E-07				14%			
docos-1-ene	222-023-7	3320-83-0	3320830	2677	Reach_1946	3900	154	-6.2	3.9E+01	1.7E+04	1.7E+03			3.5E-07	1.1E-07	3.5E-07							
692-514-2	248-503-6	27511-79-1	27511791	5810	Reach_2609	3901	350	0.0												14%			
2,6,10,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaene	203-826-1	111-02-4	111024	1536	Reach_842	3902	411	58.9	1.5E-04	3.3E-07	1.3E+14			1.1E-06	1.1E-07	3.5E-07							
(Z)-N-octadecyldocos-13-enamide	233-226-5	10094-45-8	10094458	1313	Reach_2281	3903	590	290.3	2.0E-13	9.3E-12	1.8E+17	15.1	14.3	1.1E-06	1.1E-07	3.5E-07							
O,O'-dioctadecylpentaerythritol bis(phosphite)	223-276-6	3806-34-6	3806346	2813	Reach_1993	3904	733	308.5	1.1E-14	2.0E-11	1.1E+15			1.1E-06	1.1E-07	3.5E-07							
4,4'-bis[4-[bis(2-hydroxyethyl)amino]-6-anilino-1,3,5-triazin-2-y	224-548-7	4404-43-7	4404437	641	Reach_2033	3905	917	349.8	2.6E-42	7.1E-09	1.7E+03	-0.52	10	8.4E-09	3.5E-08	1.1E-07				23%			
N,N'-(2-chloro-1,4-phenylene)bis[4-[(2,5-dichlorophenyl)azo]-3	226-106-9	5280-78-4	5280784	3075	Reach_2091	3906	829	349.8	1.2E-30	7.7E-12	1.8E+15	8.91		1.1E-07	3.5E-09	1.1E-08							
tetracosanol	208-043-9	506-51-4	506514	3014	Reach_1311	3907	355	141.0	3.2E-07	1.1E-04	4.6E+10	15.9		1.1E-06	3.5E-07	1.1E-06							
(Z)-octadec-9-enyl oleate	222-980-0	3687-45-4	3687454	2781	Reach_1981	3908	533	218.5	1.4E-09	4.5E-10	1.4E+16			1.1E-06	1.1E-07	3.5E-07							
2,2-bis[[(1-oxoisononyl)oxy]methyl]-1,3-propanediyl diisonona	298-364-0	93803-89-5	93803895	4083	Reach_2997	3909	697	253.8	6.4E-12	2.7E-09	2.0E+14			1.1E-06	1.1E-07	3.5E-07							
dihexadecyl peroxodicarbonate	247-611-0	26322-14-5	26322145	2464	Reach_2579	3910	571	245.4	2.5E-11	9.6E-10	9.5E+14			1.1E-06	1.1E-07	3.5E-07							
hexadecyl 3,5-bis-tert-butyl-4-hydroxybenzoate	267-342-2	67845-93-6	67845936	3501	Reach_2891	3911	475	219.3	1.6E-09	1.3E-06	2.1E+12	8.5		1.1E-06	1.1E-07	3.5E-07							
ditetradecyl peroxydicarbonate	258-436-4	53220-22-7	53220227	3092	Reach_2790	3912	515	215.4	9.1E-10	7.0E-08	1.0E+13			1.1E-06	1.1E-07	3.5E-07							
N,N'-phenylene-1,4-bis[4-[(2,5-dichlorophenyl)azo]-3-hydroxyr	225-730-9	5036-48-6	5036486	3003	Reach_2072	3913	125	69.7	3.1E-01	1.0E+06	1.3E+00	0		1.1E-06	1.1E-07	3.5E-07							
N,N'-(2,5-dichloro-1,4-phenylene)bis[4-[(2,5-dichlorophenyl)az	255-005-2	40618-31-3	40618313	2860	Reach_2732	3914	863	349.8	2.9E-31	1.2E-12	2.1E+15	8.84		3.5E-08	3.5E-09	1.1E-08							
(Z)-N-octadec-9-enylhexadecan-1-amide	240-367-6	16260-09-6	16260096	2086	Reach_2416	3915	506	257.8	3.5E-11	5.9E-09	2.0E+14	15.1	14.3	1.1E-06	1.1E-07	3.5E-07							
(1S)-1,5-anhydro-2,3,4,6-tetrakis-O-(2,2-dimethylpropanoyl)-1-	695-878-0	1283129-18-9	1283129189	1819	Reach_4696	3916	781	318.0	2.3E-15	6.9E-09	2.0E+11			1.1E-06	1.1E-07	3.5E-07							
618-295-5	618-295-5	897626-46-9	897626469	3984	Reach_4490	3917	749	291.3	3.9E-14	4.6E-15	2.4E+21			1.1E-06	1.1E-07	3.5E-07							
glycerol tristearate	209-097-6	555-43-1	555431	3174	Reach_1365	3918	892	349.8	2.6E-18	2.1E-18	8.7E+23			1.1E-06	1.1E-07	3.5E-07							
1-amino-4-(3-amino-2,4,6-trimethyl-5-sulphoanilino)-9,10-dihy	246-025-2	24124-40-1	24124401	2374	Reach_2539	3919	532	349.8	1.8E-24	1.2E-04	2.8E+01	-1.72	8.51	3.5E-07	3.5E-08	1.1E-07				16%			
N,N'-(2,5-dichloro-1,4-phenylene)bis[4-[[2-chloro-5-(trifluorom	257-776-0	52238-92-3	52238923	3055	Reach_2778	3920	930	349.8	3.0E-30	1.3E-13	9.3E+15	8.75		1.1E-07	3.5E-09	1.1E-08							
N,N'-naphthalene-1,5-diylbis[4-[(2,3-dichlorophenyl)azo]-3-hyc	271-178-7	68516-75-6	68516756	3519	Reach_2908	3921	845	349.8	2.1E-32	1.9E-12	2.2E+16	8.98		1.1E-07	3.5E-09	1.1E-08							
609-812-5	250-299-9	30693-53-9	30693539	5835	Reach_2649	3922	240	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				14%			
3,5-Dihydroxy-4-[3-(4-hydroxyphenyl)propanoyl]phenyl 2-O-(6	638-777-9	376348-78-6	376348786	2804	Reach_4601	3923	295	163.3	1.4E-05	1.5E+01	3.0E+02	13.5		1.1E-06	3.5E-07	1.1E-06				14%			
colchicoside	207-513-0	477-29-2	477292	2969	Reach_1290	3924	548	347.8	6.1E-23	1.1E+02	1.9E-01	14	14.7	3.5E-07	1.1E-07	3.5E-07				16%			
REACH - mono constituent organics (not on SOLUTIONS' MLoS)																							
count							*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*182*	*74*	*182*	*182*	*182*	*182*	*182*
sum																	*2.9E+06*	*5.8E+05*	*5.3E+05*	*18%*			
standard deviation																					*1.2*	*1.2*	*1.2*
2.5-p																	*1.7E+00*	*8.0E+00*	*3.1E-01*	*18%*	*-9.9*	*-10.2*	*-11.8*
50-p																	*4.9E+02*	*7.4E+02*	*8.9E+01*	*18%*	*-7.4*	*-7.7*	*-9.4*
97.5-p																	*2.9E+04*	*4.1E+04*	*5.4E+03*	*18%*	*-5.6*	*-5.9*	*-7.6*
nitrobenzene	202-716-0	98-95-3	98953	-	-	3944														18%	-3.9	-4.2	-5.8
2-hydroxy-2-methylpropionitrile	200-909-4	75-86-5	75865	-	-	3945														18%	-4.4	-4.7	-6.4
sodium formate	205-488-0	141-53-7	141537	-	-	3946														18%	-5.1	-5.4	-7.0
tris[2-[2-(2-methoxyethoxy)ethoxy]ethyl] orthoborate	250-418-4	30989-05-0	30989050	-	-	3947														18%	-5.2	-5.5	-7.1
sodium acetate	204-823-8	127-09-3	127093	-	-	3948														18%	-5.6	-5.9	-7.6
29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32 copper	205-685-1	147-14-8	147148	-	-	3949														18%	-5.6	-5.9	-7.6
triethylaluminium	202-619-3	97-93-8	97938	-	-	3950														18%	-5.7	-6.0	-7.6
benzoyl chloride	202-710-8	98-88-4	98884	-	-	3951														18%	-5.7	-6.0	-7.6
1,2-dichlorobenzene	202-425-9	95-50-1	95501	-	-	3952														18%	-5.7	-6.0	-7.7
Coke (coal), naphtha cracking ethylene manuf. by-product	305-500-5	94581-02-9	94581029	-	-	3953														18%	-5.7	-6.0	-7.7
calcium 3-hydroxy-4-[(4-methyl-2-sulphonatophenyl)azo]-2-na	226-109-5	5281-04-9	5281049	-	-	3954														18%	-5.7	-6.0	-7.7
(+)-tartaric acid	201-766-0	87-69-4	87694	-	-	3955														18%	-5.7	-6.1	-7.7
hydrazine	206-114-9	302-01-2	302012	-	-	3956														18%	-5.8	-6.1	-7.7
N,N-dimethylacetamide	204-826-4	127-19-5	127195	-	-	3957														18%	-5.8	-6.1	-7.7
tributyltin chloride	215-958-7	1461-22-9	1461229	-	-	3958														18%	-5.8	-6.1	-7.7
3,4-dichloroaniline	202-448-4	95-76-1	95761	-	-	3959														18%	-5.8	-6.1	-7.8
potassium acetate	204-822-2	127-08-2	127082	-	-	3960														18%	-6.0	-6.3	-7.9
butyllithium	203-698-7	109-72-8	109728	-	-	3961														18%	-6.0	-6.3	-7.9
triethyldialuminium trichloride	235-137-7	12075-68-2	12075682	-	-	3962														18%	-6.0	-6.4	-8.0
2-ethylhexyl 10-ethyl-4,4-dimethyl-7-oxo-8-oxa-3,5-dithia-4-sta	260-829-0	57583-35-4	57583354	-	-	3963														18%	-6.1	-6.4	-8.0

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
2-ethylhexyl 10-ethyl-4-[[2-[(2-ethylhexyl)oxy]-2-oxoethyl]thio]	260-828-5	57583-34-3	57583343	-	-	3964														18%	-6.1	-6.4	-8.0
1,2-dichloro-4-(trichloromethyl)benzene	235-869-7	13014-24-9	13014249	-	-	3965														18%	-6.1	-6.4	-8.1
pyridine-2-thiol 1-oxide, sodium salt	223-296-5	3811-73-2	3811732	-	-	3966														18%	-6.1	-6.4	-8.1
2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stan	239-622-4	15571-58-1	15571581	-	-	3967														18%	-6.2	-6.5	-8.2
tetrakis(tritolyl phosphite)nickel	252-777-2	35884-66-3	35884663	-	-	3968														18%	-6.3	-6.6	-8.2
N-vinylformamide	236-102-9	13162-05-5	13162055	-	-	3969														18%	-6.3	-6.6	-8.3
1-isopropyl-2,2-dimethyltrimethylene diisobutyrate	229-934-9	6846-50-0	6846500	-	-	3970														18%	-6.3	-6.6	-8.3
copper chlorophthalocyanine	235-476-0	12239-87-1	12239871	-	-	3971														18%	-6.4	-6.7	-8.3
sec-butyllithium	209-927-7	598-30-1	598301	-	-	3972														18%	-6.4	-6.7	-8.4
2-ethylhexyl 10-ethyl-4-[[2-[(2-ethylhexyl)oxy]-2-oxoethyl]thio]	248-227-6	27107-89-7	27107897	-	-	3973														18%	-6.4	-6.7	-8.4
tetrabutyltin	215-960-8	1461-25-2	1461252	-	-	3974														18%	-6.4	-6.7	-8.4
titanium tetraisopropanolate	208-909-6	546-68-9	546689	-	-	3975														18%	-6.4	-6.7	-8.4
methyl salicylate	204-317-7	119-36-8	119368	-	-	3976														18%	-6.5	-6.8	-8.4
dicyclohexylamine	202-980-7	101-83-7	101837	-	-	3977														18%	-6.5	-6.8	-8.4
tetraethyllead	201-075-4	78-00-2	78002	-	-	3978														18%	-6.5	-6.8	-8.4
zinc dilaurate	219-518-5	2452-01-9	2452019	-	-	3979														18%	-6.5	-6.8	-8.5
sodium diethyldithiocarbamate	205-710-6	148-18-5	148185	-	-	3980														18%	-6.5	-6.8	-8.5
n-butyltin trichloride	214-263-6	1118-46-3	1118463	-	-	3981														18%	-6.6	-6.9	-8.5
tetraoctyltin	222-733-7	3590-84-9	3590849	-	-	3982														18%	-6.6	-6.9	-8.6
sodium hydrogen di(acetate)	204-814-9	126-96-5	126965	-	-	3983														18%	-6.6	-6.9	-8.6
tert-butyl 2-ethylperoxyhexanoate	221-110-7	3006-82-4	3006824	-	-	3984														18%	-6.6	-6.9	-8.6
lithiumbis(trimethylsilyl)amide	223-725-6	4039-32-1	4039321	-	-	3985														18%	-6.6	-6.9	-8.6
bis(triphenylsilyl) chromate	216-612-8	1624-02-8	1624028	-	-	3986														18%	-6.6	-6.9	-8.6
lithium diisopropylamide	223-893-0	4111-54-0	4111540	-	-	3987														18%	-6.6	-6.9	-8.6
dichlorodioctylstannane	222-583-2	3542-36-7	3542367	-	-	3988														18%	-6.6	-7.0	-8.6
zinc bis(diethyldithiocarbamate)	238-270-9	14324-55-1	14324551	-	-	3989														18%	-6.7	-7.0	-8.6
zinc bis(dibutyldithiocarbamate)	205-232-8	136-23-2	136232	-	-	3990														18%	-6.7	-7.0	-8.7
tin bis(2-ethylhexanoate)	206-108-6	301-10-0	301100	-	-	3991														18%	-6.8	-7.1	-8.7
methoxyacetic acid	210-894-6	625-45-6	625456	-	-	3992														18%	-6.8	-7.1	-8.7
tributylaluminium	214-240-0	1116-70-7	1116707	-	-	3993														18%	-6.8	-7.1	-8.7
phenyllithium	209-720-1	591-51-5	591515	-	-	3994														18%	-6.8	-7.1	-8.8
bis(2-(2-butoxyethoxy)ethoxy)methane	205-598-9	143-29-3	143293	-	-	3995														18%	-6.8	-7.2	-8.8
2-ethylhexyl 4,4-dibutyl-10-ethyl-7-oxo-8-oxa-3,5-dithia-4-stan	234-186-1	10584-98-2	10584982	-	-	3996														18%	-6.9	-7.2	-8.8
dibutyltin oxide	212-449-1	818-08-6	818086	-	-	3997														18%	-6.9	-7.2	-8.9
ammonium acetate	211-162-9	631-61-8	631618	-	-	3998														18%	-6.9	-7.2	-8.9
dibutyltin dichloride	211-670-0	683-18-1	683181	-	-	3999														18%	-6.9	-7.3	-8.9
N-[3-(dimethylamino)propyl]methacrylamide	226-002-3	5205-93-6	5205936	-	-	4000														18%	-7.0	-7.3	-8.9
imidazole	206-019-2	288-32-4	288324	-	-	4001														18%	-7.0	-7.3	-8.9
trichlorooctylstannane	221-435-4	3091-25-6	3091256	-	-	4002														18%	-7.0	-7.3	-8.9
sodium dibenzyldithiocarbamate	259-587-9	55310-46-8	55310468	-	-	4003														18%	-7.0	-7.3	-8.9
aluminium triformate	230-898-1	7360-53-4	7360534	-	-	4004														18%	-7.0	-7.3	-9.0
sodium (S)-lactate	212-762-3	867-56-1	867561	-	-	4005														18%	-7.0	-7.3	-9.0
2-(2H-benzotriazol-2-yl)-p-cresol	219-470-5	2440-22-4	2440224	-	-	4006														18%	-7.0	-7.3	-9.0
diethylaluminium chloride	202-477-2	96-10-6	96106	-	-	4007														18%	-7.0	-7.3	-9.0
dioctyltin oxide	212-791-1	870-08-6	870086	-	-	4008														18%	-7.0	-7.3	-9.0
diethylzinc	209-161-3	557-20-0	557200	-	-	4009														18%	-7.0	-7.4	-9.0
2,4-dichloro-1-(trichloromethyl)benzene	235-868-1	13014-18-1	13014181	-	-	4010														18%	-7.1	-7.4	-9.0
diisobutylaluminium hydride	214-729-9	1191-15-7	1191157	-	-	4011														18%	-7.1	-7.4	-9.0
lead di(acetate)	206-104-4	301-04-2	301042	-	-	4012														18%	-7.1	-7.4	-9.0
benzylmagnesium chloride	230-039-0	6921-34-2	6921342	-	-	4013														18%	-7.1	-7.4	-9.1
614-695-9	614-695-9	68649-12-7	68649127	-	-	4014														18%	-7.1	-7.4	-9.1
4-(Pyridin-4-yl)-1,3-thiazole-2(3H)-thione	616-441-2	77168-63-9	77168639	-	-	4015														18%	-7.1	-7.4	-9.1
(2-hydroxyethyl)(3-hydroxypropyl)dimethylammonium chlorid	278-860-3	78182-00-0	78182000	-	-	4016														18%	-7.1	-7.4	-9.1
trichloro(chloromethyl)silane	216-316-9	1558-25-4	1558254	-	-	4017														18%	-7.1	-7.4	-9.1
2-fluorotoluene	202-428-5	95-52-3	95523	-	-	4018														18%	-7.1	-7.4	-9.1
di(morpholin-4-yl) disulphide	203-103-0	103-34-4	103344	-	-	4019														18%	-7.1	-7.4	-9.1
magnesium ethanolate	219-323-5	2414-98-4	2414984	-	-	4020														18%	-7.1	-7.4	-9.1
3-aminopropyldiethylamine	203-236-4	104-78-9	104789	-	-	4021														18%	-7.1	-7.4	-9.1
tricarbonyl(methylcyclopentadienyl)manganese	235-166-5	12108-13-3	12108133	-	-	4022														18%	-7.2	-7.5	-9.1
zinc bis[12-hydroxyoctadecanoate]	252-669-5	35674-68-1	35674681	-	-	4023														18%	-7.2	-7.5	-9.1
ferrocene	203-039-3	102-54-5	102545	-	-	4024														18%	-7.2	-7.5	-9.2
ethyl 9,9-dioctyl-4,7,11-trioxo-3,8,10-trioxa-9-stannatetradeca	268-500-3	68109-88-6	68109886	-	-	4025														18%	-7.2	-7.5	-9.2
Lead titanium zirconium oxide	235-727-4	12626-81-2	12626812	-	-	4026														18%	-7.2	-7.5	-9.2
dibutyltin dilaurate	201-039-8	77-58-7	77587	-	-	4027														18%	-7.2	-7.6	-9.2
titanium(4+) ethanolate	221-410-8	3087-36-3	3087363	-	-	4028														18%	-7.3	-7.6	-9.2
ethylaluminium dichloride	209-248-6	563-43-9	563439	-	-	4029														18%	-7.3	-7.6	-9.2
[2R-(2α,3Z,5α)]-3-(2-hydroxyethylidene)-7-oxo-4-oxa-1-azabicy	266-104-5	66069-34-9	66069349	-	-	4030														18%	-7.3	-7.6	-9.3
adipohydrazide	213-999-5	1071-93-8	1071938	-	-	4031														18%	-7.4	-7.7	-9.3
bis(2,4-dichlorobenzoyl) peroxide	205-094-9	133-14-2	133142	-	-	4032														18%	-7.4	-7.7	-9.3
sodium lactate	200-772-0	72-17-3	72173	-	-	4033														18%	-7.4	-7.7	-9.3
bismuth oxide salicylate	238-953-1	14882-18-9	14882189	-	-	4034														18%	-7.4	-7.7	-9.4
copper di(acetate)	205-553-3	142-71-2	142712	-	-	4035														18%	-7.4	-7.7	-9.4
aluminium triisopropanolate	209-090-8	555-31-7	555317	-	-	4036														18%	-7.4	-7.7	-9.4
sodium dihydridobis(2-methoxyethanolato)aluminate(1-)	245-178-2	22722-98-1	22722981	-	-	4037														18%	-7.4	-7.7	-9.4
(R*,R*)-(±)-5-amino-N,N'-bis(2,3-dihydroxypropyl)-2,4,6-triiodo	266-162-1	66108-89-2	66108892	-	-	4038														18%	-7.4	-7.7	-9.4

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
titanium(4+) 2-(dimethylamino)ethanolate	257-897-9	52406-71-0	52406710	-	-	4039														18%	-7.5	-7.8	-9.4
2,2-dioctyl-1,3,2-oxathiastannolan-5-one	239-581-2	15535-79-2	15535792	-	-	4040														18%	-7.5	-7.8	-9.5
2-(2H-benzotriazol-2-yl)-4,6-ditertpentylphenol	247-384-8	25973-55-1	25973551	-	-	4041														18%	-7.5	-7.8	-9.5
lactic acid, compound with 3-[2-(dimethylamino)ethyl] 1-(2-eth	269-358-5	68227-46-3	68227463	-	-	4042														18%	-7.5	-7.8	-9.5
magnesium di(acetate)	205-554-9	142-72-3	142723	-	-	4043														18%	-7.5	-7.8	-9.5
sodium piperidine-1-carbodithioate	212-843-3	873-57-4	873574	-	-	4044														18%	-7.5	-7.8	-9.5
titanium tetrakis(2-ethylhexanolate)	213-969-1	1070-10-6	1070106	-	-	4045														18%	-7.6	-7.9	-9.5
[1,3,8,16,18,24-hexabromo-2,4,9,10,11,15,17,22,23,25-decach	238-238-4	14302-13-7	14302137	-	-	4046														18%	-7.6	-7.9	-9.5
N-(3-aminopropyl)iminodiethanol	225-642-0	4985-85-7	4985857	-	-	4047														18%	-7.6	-7.9	-9.6
617-903-6	617-903-6	86675-46-9	86675469	-	-	4048														18%	-7.6	-7.9	-9.6
cyclohex-3-ene-1-carbaldehyde	202-858-3	100-50-5	100505	-	-	4049														18%	-7.6	-7.9	-9.6
aluminium tri-sec-butanolate	218-871-2	2269-22-9	2269229	-	-	4050														18%	-7.6	-7.9	-9.6
triisobutylaluminium	202-906-3	100-99-2	100992	-	-	4051														18%	-7.6	-7.9	-9.6
methyl (Z,Z)-8,8-dibutyl-3,6,10-trioxo-2,7,9-trioxa-8-stannatrid	239-594-3	15546-11-9	15546119	-	-	4052														18%	-7.6	-7.9	-9.6
p-methoxypropiophenone	204-512-7	121-97-1	121971	-	-	4053														18%	-7.6	-8.0	-9.6
trisodium bis[2-[[2,4-dihydroxy-3-[(2-methyl-4-sulphophenyl)a	278-145-6	75234-41-2	75234412	-	-	4054														18%	-7.7	-8.0	-9.6
phenylacetic acid	203-148-6	103-82-2	103822	-	-	4055														18%	-7.7	-8.1	-9.7
619-419-0	619-419-0	99290-97-8	99290978	-	-	4056														18%	-7.8	-8.1	-9.7
1,3-diethyldiphenylurea	201-645-2	85-98-3	85983	-	-	4057														18%	-7.8	-8.1	-9.8
trioctylaluminium	213-964-4	1070-00-4	1070004	-	-	4058														18%	-7.8	-8.1	-9.8
calcium (S)-2-hydroxypropionate	248-953-3	28305-25-1	28305251	-	-	4059														18%	-7.8	-8.1	-9.8
Phosphorous acid, tri-C12-14-alkyl esters	297-701-9	93686-48-7	93686487	-	-	4060														18%	-7.8	-8.2	-9.8
bis(ethyl acetoacetato-O1',O3)bis(2-methylpropan-1-olato)tita	281-161-6	83877-91-2	83877912	-	-	4061														18%	-7.9	-8.2	-9.8
[29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]zinc	238-262-5	14320-04-8	14320048	-	-	4062														18%	-7.9	-8.2	-9.9
bis(ethyl acetoacetato-O1',O3)bis(propan-2-olato)titanium	248-697-2	27858-32-8	27858328	-	-	4063														18%	-7.9	-8.2	-9.9
3-[(4-chloro-2-nitrophenyl)azo]-2-methylpyrazolo[5,1-b]quinaz	277-823-9	74336-59-7	74336597	-	-	4064														18%	-7.9	-8.2	-9.9
trichlorotrimethyldialuminium	235-698-8	12542-85-7	12542857	-	-	4065														18%	-7.9	-8.3	-9.9
dimethyltin dichloride	212-039-2	753-73-1	753731	-	-	4066														18%	-8.0	-8.3	-9.9
ferrate(4-), hexakis(cyano-C)-, methylated 4-[(4-aminophenyl)(	235-468-7	12237-62-6	12237626	-	-	4067														18%	-8.0	-8.3	-9.9
N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2-m	235-425-2	12225-06-8	12225068	-	-	4068														18%	-8.0	-8.3	-9.9
bismuth citrate	212-390-1	813-93-4	813934	-	-	4069														18%	-8.0	-8.3	-9.9
dibutylbis(pentane-2,4-dionato-O,O')tin	245-152-0	22673-19-4	22673194	-	-	4070														18%	-8.0	-8.3	-10.0
butylethylmagnesium	263-454-0	62202-86-2	62202862	-	-	4071														18%	-8.0	-8.3	-10.0
Octanoic acid, zinc salt, basic	291-793-4	90480-58-3	90480583	-	-	4072														18%	-8.0	-8.3	-10.0
tin(II) oxalate	212-414-0	814-94-8	814948	-	-	4073														18%	-8.0	-8.3	-10.0
Amides, tall-oil fatty, N-(hydroxyethyl)	268-950-0	68155-22-6	68155226	-	-	4074														18%	-8.1	-8.4	-10.0
Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo	276-461-9	72207-62-6	72207626	-	-	4075														18%	-8.1	-8.4	-10.0
[phthalato(2-)]dioxotrilead	273-688-5	69011-06-9	69011069	-	-	4076														18%	-8.1	-8.4	-10.0
dichloroisobutylaluminium	217-563-5	1888-87-5	1888875	-	-	4077														18%	-8.1	-8.4	-10.0
601-495-1	601-495-1	117829-74-0	117829740	-	-	4078														18%	-8.1	-8.4	-10.1
dipropylmalonic acid	216-664-1	1636-27-7	1636277	-	-	4079														18%	-8.1	-8.4	-10.1
696-062-7	696-062-7	14878-28-5	14878285	-	-	4080														18%	-8.1	-8.4	-10.1
aluminium tri(hexanolate)	245-546-2	23275-26-5	23275265	-	-	4081														18%	-8.1	-8.4	-10.1
619-741-1	619-741-1	874209-13-9	874209139	-	-	4082														18%	-8.1	-8.4	-10.1
chromium trioleate	244-256-3	21178-63-2	21178632	-	-	4083														18%	-8.1	-8.4	-10.1
3-(4-amino-2-methylpyrimidin-5-ylmethyl)-5-(2-hydroxyethyl)-4	206-077-9	299-35-4	299354	-	-	4084														18%	-8.1	-8.4	-10.1
605-753-4	605-753-4	175217-23-9	175217239	-	-	4085														18%	-8.1	-8.4	-10.1
Alkanes, C4-12	269-792-5	68333-81-3	68333813	-	-	4086														18%	-8.1	-8.4	-10.1
lead 2,4,6-trinitro-m-phenylene dioxide	239-290-0	15245-44-0	15245440	-	-	4087														18%	-8.1	-8.4	-10.1
trihexylaluminium	214-241-6	1116-73-0	1116730	-	-	4088														18%	-8.2	-8.5	-10.2
sodium 2-methylbutan-2-olate	238-639-4	14593-46-5	14593465	-	-	4089														18%	-8.2	-8.5	-10.2
trimethylaluminium	200-853-0	75-24-1	75241	-	-	4090														18%	-8.2	-8.6	-10.2
magnesium 2-methylpropan-2-olate	250-931-3	32149-57-8	32149578	-	-	4091														18%	-8.3	-8.7	-10.3
citric acid, nickel salt	245-119-0	22605-92-1	22605921	-	-	4092														18%	-8.5	-8.8	-10.5
606-280-6	606-280-6	192704-54-4	192704544	-	-	4093														18%	-8.6	-8.9	-10.6
dibutoxydibutylstannane	222-103-1	3349-36-8	3349368	-	-	4094														18%	-8.6	-8.9	-10.6
dibutyldimethoxystannane	213-935-6	1067-55-6	1067556	-	-	4095														18%	-8.6	-8.9	-10.6
4-amino-6-[(E)-{5-[(4-chloro-6-{ethyl[3-(vinylsulfonyl)phenyl]ar	700-419-5	1177247-66-3	1177247663	-	-	4096														18%	-8.7	-9.0	-10.6
dibutyltin maleate	201-077-5	78-04-6	78046	-	-	4097														18%	-8.7	-9.0	-10.7
3-hydroxy-4'-methoxy-2-naphthanilide	202-190-2	92-79-5	92795	-	-	4098														18%	-8.7	-9.0	-10.7
chromium triacetate	213-909-4	1066-30-4	1066304	-	-	4099														18%	-8.8	-9.1	-10.7
bis(tributyltin) oxide	200-268-0	56-35-9	56359	-	-	4100														18%	-8.8	-9.1	-10.8
methylmagnesium chloride	211-629-7	676-58-4	676584	-	-	4101														18%	-8.8	-9.1	-10.8
[2-{[(2-{3-[(4-{ethyl[3-(vinylsulfonyl)phenyl]amino}-6-fluoro-1,3	700-687-3	1291070-04-6	1291070046	-	-	4102														18%	-8.9	-9.2	-10.8
diethyl ethyl(1-methylbutyl)malonate	200-981-7	76-72-2	76722	-	-	4103														18%	-8.9	-9.2	-10.9
disodium hydrogen bis[3-hydroxy-4-[(2-hydroxy-1-naphthyl)azo	235-628-6	12392-64-2	12392642	-	-	4104														18%	-8.9	-9.2	-10.9
trisodium [3-{(E)-[4-{[6-anilino-1-(hydroxy-κO)-3-sulfo-2-naphtl	616-328-8	76359-37-0	76359370	-	-	4105														18%	-9.1	-9.4	-11.1
bis[1-carbamimidoyl-kN'-urea-kO)]copper(2+) dinitrate	800-038-5	1071838-81-7	1071838817	-	-	4106														18%	-9.1	-9.4	-11.1
Magnesium bis(2-ethylbutanoate)	700-021-1	79992-76-0	79992760	-	-	4107														18%	-9.1	-9.5	-11.1
4-[(4-chloro-2-nitrophenyl)azo]-3-hydroxy-N-(2-methylphenyl)(	229-314-8	6471-50-7	6471507	-	-	4108														18%	-9.2	-9.5	-11.1
nickel(2+) hydrogen citrate	242-533-3	18721-51-2	18721512	-	-	4109														18%	-9.2	-9.5	-11.1
cobalt(2+) hydrogen citrate	242-538-0	18727-04-3	18727043	-	-	4110														18%	-9.2	-9.5	-11.1
aluminium tris(2,4-pentanedionato-O,O')	237-741-6	13963-57-0	13963570	-	-	4111														18%	-9.2	-9.5	-11.2
hydrogen [1-[(2-hydroxy-4-nitrophenyl)azo]-2-naphtholato(2-)]	257-804-1	52277-71-1	52277711	-	-	4112														18%	-9.2	-9.5	-11.2
Solvate of methyl 1-C-[4-chloro-3-(4-ethoxybenzyl)phenyl]-β-D-	619-496-0	960404-59-5	960404595	-	-	4113														18%	-9.2	-9.5	-11.2

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Magnesium bis(2-ethylhexan-1-olate)	805-232-3	98906-78-6	98906786	-	-	4114														18%	-9.3	-9.6	-11.3
1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthyl)ethan	244-240-6	21145-77-7	21145777	-	-	4115														18%	-9.4	-9.7	-11.4
chloro(1-methylethyl)magnesium	213-947-1	1068-55-9	1068559	-	-	4116														18%	-9.5	-9.8	-11.5
pyridinium dichromate	243-478-8	20039-37-6	20039376	-	-	4117														18%	-9.7	-10.0	-11.7
trinickel dicitrate	227-873-2	6018-92-4	6018924	-	-	4118														18%	-9.7	-10.0	-11.7
(6R,6'S)-6,6'-ethane-1,2-diylbis(6H-dibenzo[c,e][1,2]oxaphosph	700-929-8	1337918-51-0	1337918510	-	-	4119														18%	-9.7	-10.1	-11.7
sodium bis[N-[7-hydroxy-8-[[2-hydroxy-5-[(methylamino)sulph	273-454-2	68966-87-0	68966870	-	-	4120														18%	-9.8	-10.1	-11.7
Acetic acid, chromium salt, basic	254-447-3	39430-51-8	39430518	-	-	4121														18%	-10.0	-10.3	-12.0
sodium hydrogen (3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)p	700-812-1	1189052-95-6	1189052956	-	-	4122														18%	-10.1	-10.4	-12.1
2-ethylhexyl lactate	228-503-2	6283-86-9	6283869	-	-	4123														18%	-10.1	-10.4	-12.1
612-411-8	612-411-8	61813-75-0	61813750	-	-	4124														18%	-10.2	-10.5	-12.1
tricobalt dicitrate	212-751-3	866-81-9	866819	-	-	4125														18%	-10.5	-10.8	-12.4
REACH - UVCB organics (not on SOLUTIONS' MLoS)																							
count							*1*	*1*	*1*	*1*	*1*	*1*	*1*	*1*	*1*	*1*	*1144*	*765*	*1144*	*1144*	*1144*	*1144*	*1144*
sum																	*5.4E+07*	*3.3E+07*	*1.0E+07*	*18%*			
standard deviation																					*1.1*	*1.1*	*1.1*
2.5-p																	*6.6E+00*	*1.1E+01*	*1.2E+00*	*18%*	*-9.3*	*-9.6*	*-11.2*
50-p																	*9.1E+02*	*8.9E+02*	*1.7E+02*	*18%*	*-7.1*	*-7.4*	*-9.1*
97.5-p																	*2.8E+05*	*2.2E+05*	*5.1E+04*	*18%*	*-4.7*	*-5.0*	*-6.6*
Fatty acids, C16-18 and C18-unsatd., Me esters	267-015-4	67762-38-3	67762383	-	-	4127														18%	-3.2	-3.5	-5.1
Fatty acids, vegetable-oil, Me esters	273-606-8	68990-52-3	68990523	-	-	4128														18%	-3.2	-3.6	-5.2
618-882-6	618-882-6	928771-01-1	928771011	-	-	4129														18%	-3.4	-3.7	-5.3
Hydrocarbons, C4	289-339-5	87741-01-3	87741013	-	-	4130														18%	-3.5	-3.8	-5.4
Fatty acids, C14-18 and C16-18-unsatd., Me esters	267-007-0	67762-26-9	67762269	-	-	4131														18%	-3.7	-4.0	-5.7
Light oil (coal), coke-oven	266-012-5	65996-78-3	65996783	-	-	4132														18%	-3.8	-4.1	-5.7
Fatty acids, C10-18 and C12-22-unsatd., C14-18 and C16-18-un	285-200-8	85049-31-6	85049316	-	-	4133														18%	-3.9	-4.2	-5.8
Tar, coal, high-temp.	266-024-0	65996-89-6	65996896	-	-	4134														18%	-3.9	-4.2	-5.9
Hydrocarbons, C3-4	270-681-9	68476-40-4	68476404	-	-	4135														18%	-4.0	-4.3	-6.0
Pitch, coal tar, high-temp.	266-028-2	65996-93-2	65996932	-	-	4136														18%	-4.1	-4.4	-6.0
Formaldehyde, oligomeric reaction products with aniline and p	500-079-6	32055-14-4	32055144	-	-	4137														18%	-4.1	-4.4	-6.0
Petroleum gases, liquefied, sweetened	270-705-8	68476-86-8	68476868	-	-	4138														18%	-4.1	-4.4	-6.0
Formaldehyde, oligomeric reaction products with aniline	500-036-1	25214-70-4	25214704	-	-	4139														18%	-4.2	-4.5	-6.2
Charcoal	240-383-3	16291-96-6	16291966	4995	PharmaBeta_418	4140	16	-152.9	7.1E+07	2.6E+03	6.0E+00	0	0	3.5E-09	3.5E-09	3.5E-09				24%	-7.3	-6.6	-9.2
Benzene, C10-13-alkyl derivs.	267-051-0	67774-74-7	67774747	-	-	4141														18%	-4.3	-4.6	-6.3
Naphtha (petroleum), light steam-cracked, thermally treated	308-714-7	98219-47-7	98219477	-	-	4142														18%	-4.3	-4.6	-6.3
m-tolylidene diisocyanate	247-722-4	26471-62-5	26471625	-	-	4143														18%	-4.3	-4.7	-6.3
dinitrotoluene	246-836-1	25321-14-6	25321146	-	-	4144														18%	-4.4	-4.7	-6.4
Benzenesulfonic acid, 4-C10-13-sec-alkyl derivs.	287-494-3	85536-14-7	85536147	-	-	4145														18%	-4.4	-4.8	-6.4
Distillates (coal tar), heavy oils	292-607-4	90640-86-1	90640861	-	-	4146														18%	-4.5	-4.8	-6.4
Tall oil, sodium salt	266-037-1	65997-01-5	65997015	-	-	4147														18%	-4.5	-4.8	-6.4
Alcohols, C12-14, ethoxylated, sulfates, sodium salts	500-234-8	68891-38-3	68891383	-	-	4148														18%	-4.5	-4.8	-6.4
diaminotoluene	246-910-3	25376-45-8	25376458	-	-	4149														18%	-4.5	-4.8	-6.5
Naphtha (petroleum), light steam-cracked, debenzenized	271-266-5	68527-26-4	68527264	-	-	4150														18%	-4.5	-4.8	-6.5
Alcohols, C12-14, ethoxylated	500-213-3	68439-50-9	68439509	-	-	4151														18%	-4.5	-4.9	-6.5
Rosin	232-475-7	8050-09-7	8050097	-	-	4152														18%	-4.6	-4.9	-6.5
Distillates (coal tar), naphthalene oils	283-484-8	84650-04-4	84650044	-	-	4153														18%	-4.6	-4.9	-6.5
Tall-oil pitch	232-414-4	8016-81-7	8016817	-	-	4154														18%	-4.6	-4.9	-6.6
Ascophyllum nodosum, ext.	283-907-6	84775-78-0	84775780	-	-	4155														18%	-4.7	-5.0	-6.6
Shale oils	269-646-0	68308-34-9	68308349	-	-	4156														18%	-4.7	-5.0	-6.6
Fatty acids, C16-18	266-928-5	67701-03-5	67701035	-	-	4157														18%	-4.7	-5.0	-6.6
308065-15-8	629-776-4	308065-15-8	308065158	-	-	4158														18%	-4.7	-5.0	-6.7
Benzenesulfonic acid, C10-13-alkyl derivs., sodium salts	270-115-0	68411-30-3	68411303	-	-	4159														18%	-4.7	-5.0	-6.7
Alkenes, C10-13	287-479-1	85535-87-1	85535871	-	-	4160														18%	-4.8	-5.1	-6.7
Hydrocarbons, C5-8	295-762-6	92128-65-9	92128659	-	-	4161														18%	-4.8	-5.1	-6.7
Anthracene oil	292-602-7	90640-80-5	90640805	-	-	4162														18%	-4.8	-5.1	-6.7
Fatty acids, C8-18 and C18-unsatd., Me esters	267-014-9	67762-37-2	67762372	-	-	4163														18%	-4.8	-5.1	-6.8
Lubricating oils, used	274-635-9	70514-12-4	70514124	-	-	4164														18%	-4.8	-5.1	-6.8
Wheat, ext., hydrolyzed	309-358-5	100209-50-5	100209505	-	-	4165														18%	-4.9	-5.2	-6.8
1,2-Benzenedicarboxylic acid, di-C9-11-branched alkyl esters, C	271-091-4	68515-49-1	68515491	-	-	4166														18%	-4.9	-5.2	-6.9
Tall oil	232-304-6	8002-26-4	8002264	-	-	4167														18%	-4.9	-5.2	-6.9
Alcohols, C9-11-iso-, C10-rich	271-234-0	68526-85-2	68526852	-	-	4168														18%	-4.9	-5.3	-6.9
Charcoal, coconut shell	271-974-4	68647-86-9	68647869	-	-	4169														18%	-5.0	-5.3	-7.0
1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C	271-090-9	68515-48-0	68515480	-	-	4170														18%	-5.0	-5.3	-7.0
Fatty acids, C14-18 and C16-18-unsatd.	266-930-6	67701-06-8	67701068	-	-	4171														18%	-5.1	-5.4	-7.0
Creosote oil, acenaphthene fraction	292-605-3	90640-84-9	90640849	-	-	4172														18%	-5.1	-5.4	-7.0
Alcohols, C8-10-iso-, C9-rich	271-233-5	68526-84-1	68526841	-	-	4173														18%	-5.1	-5.4	-7.0
Corn, steep liquor	266-113-4	66071-94-1	66071941	-	-	4174														18%	-5.1	-5.4	-7.0
Syrups, corn, hydrogenated	270-337-8	68425-17-2	68425172	-	-	4175														18%	-5.1	-5.4	-7.0
Dec-1-ene, homopolymer, hydrogenated Dec-1-ene, oligomers,	500-183-1	68037-01-4	68037014	-	-	4176														18%	-5.1	-5.4	-7.0
Benzene, (1-methylethyl)-, oxidized, polyphenyl residues	269-798-8	68333-89-1	68333891	-	-	4177														18%	-5.1	-5.4	-7.1
Alkanes, C14-17, chloro	287-477-0	85535-85-9	85535859	-	-	4178														18%	-5.1	-5.4	-7.1
Distillates (petroleum), steam-cracked	265-194-3	64742-91-2	64742912	-	-	4179														18%	-5.1	-5.4	-7.1
Tar, brown-coal, low-temp.	309-886-6	101316-84-1	101316841	-	-	4180														18%	-5.1	-5.4	-7.1
Sucrose, propoxylated	500-029-3	9049-71-2	9049712	-	-	4181														18%	-5.1	-5.4	-7.1

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
vinyl neodecanoate	256-905-8	51000-52-3	51000523	-	-	4182														18%	-5.1	-5.4	-7.1
629-693-3	629-693-3	740817-83-8	740817838	-	-	4183														18%	-5.2	-5.5	-7.1
Fatty acids, C6-24 and C6-24-unsatd., Me esters, distn. residues	310-083-8	102242-52-4	102242524	-	-	4184														18%	-5.2	-5.5	-7.1
D-Glucitol, propoxylated	500-118-7	52625-13-5	52625135	-	-	4185														18%	-5.2	-5.5	-7.1
Hydrocarbons, C5, ethylene-manuf.-by-product, hydrogenated	295-765-2	92128-68-2	92128682	-	-	4186														18%	-5.2	-5.5	-7.1
Glycerol, propoxylated	500-044-5	25791-96-2	25791962	-	-	4187														18%	-5.2	-5.5	-7.1
615-494-9	615-494-9	71808-39-4	71808394	-	-	4188														18%	-5.2	-5.5	-7.2
Amines, C12-14-alkyldimethyl	283-464-9	84649-84-3	84649843	-	-	4189														18%	-5.2	-5.5	-7.2
Soybean oil, epoxidized	232-391-0	8013-07-8	8013078	-	-	4190														18%	-5.2	-5.5	-7.2
Fatty acids, C18-unsatd., dimers	500-148-0	61788-89-4	61788894	-	-	4191														18%	-5.3	-5.6	-7.2
Ethers, C5-6-branched alkyl Me	295-322-3	91995-60-7	91995607	-	-	4192														18%	-5.3	-5.6	-7.2
Pitch, petroleum, arom.	269-110-6	68187-58-6	68187586	-	-	4193														18%	-5.3	-5.6	-7.3
Distillates (petroleum), C3-6, piperylene-rich	270-726-2	68477-35-0	68477350	-	-	4194														18%	-5.3	-5.6	-7.3
(1-methyl-1,2-ethanediyl)bis[oxy(methyl-2,1-ethanediyl)] diacr	256-032-2	42978-66-5	42978665	-	-	4195														18%	-5.3	-5.6	-7.3
Butene, homopolymer (products derived from either/or But-1-	500-004-7	9003-29-6	9003296	-	-	4196														18%	-5.3	-5.6	-7.3
Cyclohexane, oxidized, aq. ext.	272-810-4	68915-38-8	68915388	-	-	4197														18%	-5.3	-5.7	-7.3
Fatty acids, C8-18 and C18-unsatd.	266-929-0	67701-05-7	67701057	-	-	4198														18%	-5.4	-5.7	-7.3
Turpentine, oil	232-350-7	8006-64-2	8006642	-	-	4199														18%	-5.4	-5.7	-7.3
Sulfuric acid, mono-C12-14-alkyl esters, sodium salts	287-809-4	85586-07-8	85586078	-	-	4200														18%	-5.4	-5.7	-7.3
Benzene, mono-C10-13-alkyl derivs., distn. residues	284-660-7	84961-70-6	84961706	-	-	4201														18%	-5.4	-5.7	-7.3
isotridecan-1-ol	248-469-2	27458-92-0	27458920	-	-	4202														18%	-5.4	-5.7	-7.3
Distillates (coal tar), benzole fraction	283-482-7	84650-02-2	84650022	-	-	4203														18%	-5.4	-5.7	-7.3
Fatty acids, C8-10, Me esters	287-636-4	85566-26-3	85566263	-	-	4204														18%	-5.4	-5.7	-7.4
Resin acids and Rosin acids, esters with pentaerythritol	232-479-9	8050-26-8	8050268	-	-	4205														18%	-5.4	-5.7	-7.4
Distillates (coal tar), light oils	283-483-2	84650-03-3	84650033	-	-	4206														18%	-5.4	-5.7	-7.4
Alcohols, C12-13, branched and linear, ethoxylated, sulfates, sc	500-513-4	161074-79-9	161074799	-	-	4207														18%	-5.4	-5.7	-7.4
Fatty acids, C8-10	273-086-2	68937-75-7	68937757	-	-	4208														18%	-5.4	-5.7	-7.4
Dodecene, branched	306-479-5	97280-83-6	97280836	-	-	4209														18%	-5.4	-5.7	-7.4
Fatty acids, C16-18, zinc salts	293-049-4	91051-01-3	91051013	-	-	4210														18%	-5.4	-5.7	-7.4
1234694-02-0	629-780-6	1234694-02-0	1234694020	-	-	4211														18%	-5.4	-5.7	-7.4
1,2-Dihydro-2,2,4-trimethylquinoline, oligomers	500-051-3	26780-96-1	26780961	-	-	4212														18%	-5.4	-5.8	-7.4
620-174-7	620-174-7	1079184-43-2	1079184432	-	-	4213														18%	-5.4	-5.8	-7.4
(2-methoxymethylethoxy)propanol	252-104-2	34590-94-8	34590948	-	-	4214														18%	-5.5	-5.8	-7.4
Fatty acids, tall-oil, low-boiling	266-039-2	65997-03-7	65997037	-	-	4215														18%	-5.5	-5.8	-7.4
Sulfonic acids, C14-17-sec-alkane, sodium salts	307-055-2	97489-15-1	97489151	-	-	4216														18%	-5.5	-5.8	-7.4
4,4'-Methylenediphenyl diisocyanate, oligomers	500-040-3	25686-28-6	25686286	-	-	4217														18%	-5.5	-5.8	-7.4
citral	226-394-6	5392-40-5	5392405	-	-	4218														18%	-5.5	-5.8	-7.4
Phenol, dodecyl-, branched	310-154-3	121158-58-5	121158585	-	-	4219														18%	-5.5	-5.8	-7.5
Glycerides, C16-18	268-084-3	68002-71-1	68002711	-	-	4220														18%	-5.5	-5.8	-7.5
Extracts, coal tar oil alk.	266-017-2	65996-83-0	65996830	-	-	4221														18%	-5.5	-5.8	-7.5
Carboxylic acids, di-, C4-6	271-678-5	68603-87-2	68603872	-	-	4222														18%	-5.5	-5.8	-7.5
Phenol, dodecyl-, sulfurized, carbonates, calcium salts, overbas	272-234-3	68784-26-9	68784269	-	-	4223														18%	-5.5	-5.8	-7.5
Rosin, fumarated	266-040-8	65997-04-8	65997048	-	-	4224														18%	-5.5	-5.8	-7.5
Alcohols, C13-15-branched and linear	287-625-4	85566-16-1	85566161	-	-	4225														18%	-5.5	-5.8	-7.5
Anthracene oil, anthracene paste	292-603-2	90640-81-6	90640816	-	-	4226														18%	-5.5	-5.9	-7.5
Resin acids and Rosin acids, esters with glycerol	232-482-5	8050-31-5	8050315	-	-	4227														18%	-5.5	-5.9	-7.5
692-061-0	692-061-0	1207435-39-9	1207435399	-	-	4228														18%	-5.6	-5.9	-7.5
Alcohols, C12-13, branched and linear, ethoxylated	500-457-0	160901-19-9	160901199	-	-	4229														18%	-5.6	-5.9	-7.5
Fatty acids, C16-18 and C18-unsatd., branched and linear	273-295-9	68955-98-6	68955986	-	-	4230														18%	-5.6	-5.9	-7.5
Nonene, branched	306-492-6	97280-95-0	97280950	-	-	4231														18%	-5.6	-5.9	-7.5
Alkenes, C20-24 α-	300-202-1	93924-10-8	93924108	-	-	4232														18%	-5.6	-5.9	-7.6
Formaldehyde, oligomeric reaction products with 1-chloro-2,3-	500-006-8	9003-36-5	9003365	-	-	4233														18%	-5.6	-5.9	-7.6
Alcohols, C12-13	278-306-0	75782-86-4	75782864	-	-	4234														18%	-5.6	-5.9	-7.6
Fatty acids, C12-18 and C18-unsatd., 2-sulfoethyl esters, sodiur	287-024-7	85408-62-4	85408624	-	-	4235														18%	-5.6	-5.9	-7.6
Amines, polyethylenepoly-, triethylenetetramine fraction	292-588-2	90640-67-8	90640678	-	-	4236														18%	-5.6	-5.9	-7.6
Orange, sweet, ext.	232-433-8	8028-48-6	8028486	-	-	4237														18%	-5.6	-5.9	-7.6
Fatty acids, C12-18	266-925-9	67701-01-3	67701013	-	-	4238														18%	-5.6	-5.9	-7.6
Fatty acids, C8-18	292-769-6	90990-08-2	90990082	-	-	4239														18%	-5.6	-5.9	-7.6
hexabromocyclododecane	247-148-4	25637-99-4	25637994	-	-	4240														18%	-5.6	-5.9	-7.6
Methyl dodec-9-enoate	700-618-7	39202-17-0	39202170	-	-	4241														18%	-5.6	-5.9	-7.6
tert-dodecanethiol	246-619-1	25103-58-6	25103586	-	-	4242														18%	-5.6	-5.9	-7.6
Alcohols, C12-15-branched and linear	292-334-0	90604-40-3	90604403	-	-	4243														18%	-5.6	-6.0	-7.6
Resin acids and Rosin acids, sodium salts	263-144-5	61790-51-0	61790510	-	-	4244														18%	-5.7	-6.0	-7.6
ethanol, 2-butoxy-, manufacture of, by-products from	310-287-7	161907-77-3	161907773	-	-	4245														18%	-5.7	-6.0	-7.6
629-695-4	629-695-4	164383-22-6	164383226	-	-	4246														18%	-5.7	-6.0	-7.6
2-Oxetanone, 3-C12-16-alkyl-4-C13-17-alkylidene derivs.	284-932-5	84989-41-3	84989413	-	-	4247														18%	-5.7	-6.0	-7.6
Fatty acids, C16-18, Me esters	287-824-6	85586-21-6	85586216	-	-	4248														18%	-5.7	-6.0	-7.6
2,5-Furandione, dihydro-, mono-C15-20-alkenyl derivs.	272-221-2	68784-12-3	68784123	-	-	4249														18%	-5.7	-6.0	-7.6
Castor oil, hydrogenated	232-292-2	8001-78-3	8001783	-	-	4250														18%	-5.7	-6.0	-7.6
Sugar, invert	232-393-1	8013-17-0	8013170	-	-	4251														18%	-5.7	-6.0	-7.6
Alcohols, C9-11	266-367-6	66455-17-2	66455172	-	-	4252														18%	-5.7	-6.0	-7.7
Fatty acids, essential, Et esters	293-054-1	91051-05-7	91051057	-	-	4253														18%	-5.7	-6.0	-7.7
Resin acids and Rosin acids, fumarated, esters with pentaerythr	305-514-1	94581-15-4	94581154	-	-	4254														18%	-5.7	-6.0	-7.7
Amines, C16-18 and C18-unsatd. alkyl	268-219-6	68037-95-6	68037956	-	-	4255														18%	-5.7	-6.0	-7.7
Alcohols, C11-14-iso-, C13-rich	271-235-6	68526-86-3	68526863	-	-	4256														18%	-5.7	-6.0	-7.7

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Octene, hydroformylation products, high-boiling	271-237-7	68526-89-6	68526896	-	-	4257														18%	-5.7	-6.0	-7.7
Octene, hydroformylation products, low-boiling	273-110-1	68938-03-4	68938034	-	-	4258														18%	-5.7	-6.0	-7.7
Glycerides, C8-18 and C18-unsatd.	266-946-3	67701-28-4	67701284	-	-	4259														18%	-5.7	-6.0	-7.7
692-840-5	692-840-5	1345668-40-7	1345668407	-	-	4260														18%	-5.7	-6.0	-7.7
Sulfonic acids, C10-21-alkane, Ph esters	293-728-5	91082-17-6	91082176	-	-	4261														18%	-5.7	-6.0	-7.7
Amines, C16-18-alkyl	292-550-5	90640-32-7	90640327	-	-	4262														18%	-5.7	-6.1	-7.7
Paraffin waxes and Hydrocarbon waxes, chloro	264-150-0	63449-39-8	63449398	-	-	4263														18%	-5.8	-6.1	-7.7
3(or 4)-methylbenzene-1,2-diamine	248-145-0	26966-75-6	26966756	-	-	4264														18%	-5.8	-6.1	-7.7
Paraffin waxes and Hydrocarbon waxes, chloro, sulfochlorinate	269-145-7	68188-19-2	68188192	-	-	4265														18%	-5.8	-6.1	-7.7
Hydrocarbons, C14-30, olefin-rich	271-036-4	68514-35-2	68514352	-	-	4266														18%	-5.8	-6.1	-7.8
Cyclohexane, oxidized, non-acidic by-products, distn. residues	271-816-4	68609-04-1	68609041	-	-	4267														18%	-5.8	-6.1	-7.8
Cyclohexane, oxidized, aq. ext., sodium salt	272-812-5	68915-39-9	68915399	-	-	4268														18%	-5.8	-6.1	-7.8
Fatty acids, C8-24	275-164-1	71076-48-7	71076487	-	-	4269														18%	-5.8	-6.1	-7.8
Naphtha, thermal cracked, residues, naphthalene cut	285-562-7	85117-10-8	85117108	-	-	4270														18%	-5.8	-6.1	-7.8
Alkenes, C9-13-branched, C10-rich	295-253-9	91994-95-5	91994955	-	-	4271														18%	-5.8	-6.1	-7.8
Alkenes, C7-9-branched, C8-rich	307-300-3	97593-00-5	97593005	-	-	4272														18%	-5.8	-6.1	-7.8
bis(nonylphenyl)amine	253-249-4	36878-20-3	36878203	-	-	4273														18%	-5.8	-6.1	-7.8
Glycerides, C16-18 mono- and di-	286-490-9	85251-77-0	85251770	-	-	4274														18%	-5.8	-6.1	-7.8
Creosote oil	263-047-8	61789-28-4	61789284	-	-	4275														18%	-5.8	-6.1	-7.8
Hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene	297-629-8	93685-81-5	93685815	-	-	4276														18%	-5.8	-6.1	-7.8
Anthracene oil, anthracene-low	292-604-8	90640-82-7	90640827	-	-	4277														18%	-5.8	-6.1	-7.8
2-Propenoic acid, 2-methyl-, C12-15-branched and linear alkyl	292-122-8	90552-02-6	90552026	-	-	4278														18%	-5.8	-6.1	-7.8
Ethylenediamine, propoxylated	500-035-6	25214-63-5	25214635	-	-	4279														18%	-5.8	-6.1	-7.8
1-Propene, chlorinated, epoxidized, distn. residues	304-800-3	94279-54-6	94279546	-	-	4280														18%	-5.8	-6.2	-7.8
Alcohols, C7-9-iso-, C8-rich	271-231-4	68526-83-0	68526830	-	-	4281														18%	-5.8	-6.2	-7.8
nitrotoluene	215-311-9	1321-12-6	1321126	-	-	4282														18%	-5.8	-6.2	-7.8
Distillates (coal tar)	266-027-7	65996-92-1	65996921	-	-	4283														18%	-5.8	-6.2	-7.8
Pitch, coal tar, high-temp., heat-treated	310-162-7	121575-60-8	121575608	-	-	4284														18%	-5.8	-6.2	-7.8
Pentanol, branched and linear	305-536-1	94624-12-1	94624121	-	-	4285														18%	-5.9	-6.2	-7.8
4,4'-Methylenediphenyl diisocyanate, oligomeric reaction prod	500-270-4	88288-99-7	88288997	-	-	4286														18%	-5.9	-6.2	-7.8
627-132-7	627-132-7	1227096-04-9	1227096049	-	-	4287														18%	-5.9	-6.2	-7.8
Poly(oxy-1,2-ethanediyl), α-butyl-ω-hydroxy-	500-012-0	9004-77-7	9004777	-	-	4288														18%	-5.9	-6.2	-7.8
600-975-8	600-975-8	110615-47-9	110615479	-	-	4289														18%	-5.9	-6.2	-7.8
Glycerides, mixed decanoyl and octanoyl	277-452-2	73398-61-5	73398615	-	-	4290														18%	-5.9	-6.2	-7.9
methacrylic acid, monoester with propane-1,2-diol	248-666-3	27813-02-1	27813021	-	-	4291														18%	-5.9	-6.2	-7.9
D-Glucopyranose, oligomers, decyl octyl glycosides	500-220-1	68515-73-1	68515731	-	-	4292														18%	-5.9	-6.2	-7.9
Tar acids, coal, crude	266-019-3	65996-85-2	65996852	-	-	4293														18%	-5.9	-6.2	-7.9
Sulfuric acid, mono-C12-18-alkyl esters, sodium salts	273-257-1	68955-19-1	68955191	-	-	4294														18%	-5.9	-6.2	-7.9
1,2-Benzenedicarboxylic acid, benzyl C7-9-branched and linear	271-082-5	68515-40-2	68515402	-	-	4295														18%	-5.9	-6.2	-7.9
4,4'-Isopropylidenediphenol, oligomeric reaction products with	500-130-2	55818-57-0	55818570	-	-	4296														18%	-5.9	-6.2	-7.9
Phenol, isopropylated	291-826-2	90480-88-9	90480889	-	-	4297														18%	-5.9	-6.2	-7.9
614-144-2	614-144-2	67800-94-6	67800946	-	-	4298														18%	-5.9	-6.2	-7.9
Fatty acids, C16-18, esters with ethylene glycol	292-932-1	91031-31-1	91031311	-	-	4299														18%	-5.9	-6.3	-7.9
Fatty acids, tall-oil, reaction products with diethylenetriamine,	273-601-0	68990-47-6	68990476	-	-	4300														18%	-6.0	-6.3	-7.9
Amines, polyethylenepoly-	268-626-9	68131-73-7	68131737	-	-	4301														18%	-6.0	-6.3	-7.9
Propylidynetrimethanol, propoxylated	500-041-9	25723-16-4	25723164	-	-	4302														18%	-6.0	-6.3	-7.9
Amines, C20-22-alkyldimethyl	296-866-4	93164-85-3	93164853	-	-	4303														18%	-6.0	-6.3	-7.9
Amines, polyethylenepoly-, tetraethylenepentamine fraction	292-587-7	90640-66-7	90640667	-	-	4304														18%	-6.0	-6.3	-7.9
pentene	246-916-6	25377-72-4	25377724	-	-	4305														18%	-6.0	-6.3	-7.9
Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethy	270-128-1	68411-46-1	68411461	-	-	4306														18%	-6.0	-6.3	-7.9
Fatty acids, C14-18 and C16-18 unsatd., triesters with trimethyl	268-093-2	68002-79-9	68002799	-	-	4307														18%	-6.0	-6.3	-7.9
Hydrocarbons, C5-rich, dicyclopentadiene-contg.	310-013-6	102110-15-6	102110156	-	-	4308														18%	-6.0	-6.3	-7.9
Tar acids, brown-coal gasification	295-536-7	92062-22-1	92062221	-	-	4309														18%	-6.0	-6.3	-7.9
Oils, vegetable, deodorizer distillates	270-700-0	68476-80-2	68476802	-	-	4310														18%	-6.0	-6.3	-7.9
Glycerides, C16-18 mono-	293-208-8	91052-47-0	91052470	-	-	4311														18%	-6.0	-6.3	-7.9
Oils, fish, oxidized, bisulfited, sodium salts	307-037-4	97488-98-7	97488987	-	-	4312														18%	-6.0	-6.3	-8.0
2,2'-Iminodiethanol, propoxylated	500-085-9	35176-06-8	35176068	-	-	4313														18%	-6.0	-6.3	-8.0
Resin acids and Rosin acids, potassium salts	263-142-4	61790-50-9	61790509	-	-	4314														18%	-6.0	-6.3	-8.0
Acetic acid, oxo-, sodium salt, reaction products with ethylenec	283-044-5	84539-55-9	84539559	-	-	4315														18%	-6.0	-6.3	-8.0
Glycerol, propoxylated, esters with acrylic acid	500-114-5	52408-84-1	52408841	-	-	4316														18%	-6.0	-6.3	-8.0
Fatty acids, C18-unsatd.	289-450-9	88895-93-6	88895936	-	-	4317														18%	-6.0	-6.3	-8.0
Resin acids and Rosin acids, calcium salts	232-694-8	9007-13-0	9007130	-	-	4318														18%	-6.0	-6.3	-8.0
Phenol, isopropylated, phosphate (3:1)	273-066-3	68937-41-7	68937417	-	-	4319														18%	-6.0	-6.3	-8.0
Ethane- 1,2-diol, propoxylated	500-078-0	31923-84-9	31923849	-	-	4320														18%	-6.0	-6.3	-8.0
Oxirane, reaction products with ammonia, distn. residues	273-224-1	68953-70-8	68953708	-	-	4321														18%	-6.0	-6.3	-8.0
Fatty acids, C16-18, esters with pentaerythritol	285-547-5	85116-93-4	85116934	-	-	4322														18%	-6.0	-6.3	-8.0
Extract residues (coal), light oil alk., acid ext., indene fraction	309-867-2	101316-62-5	101316625	-	-	4323														18%	-6.0	-6.3	-8.0
Propylidynetrimethanol, ethoxylated, esters with acrylic acid	500-066-5	28961-43-5	28961435	-	-	4324														18%	-6.0	-6.4	-8.0
1,4-Benzenedicarboxylic acid, dimethyl ester, manuf. of, by-pro	273-521-6	68988-22-7	68988227	-	-	4325														18%	-6.0	-6.4	-8.0
Montan wax	232-313-5	8002-53-7	8002537	-	-	4326														18%	-6.1	-6.4	-8.0
isooctadecanoic acid	250-178-0	30399-84-9	30399849	-	-	4327														18%	-6.1	-6.4	-8.0
Polysulfides, di-tert-Bu	273-103-3	68937-96-2	68937962	-	-	4328														18%	-6.1	-6.4	-8.0
Solvent naphtha (coal), xylene-styrene cut	287-502-5	85536-20-5	85536205	-	-	4329														18%	-6.1	-6.4	-8.0
1,2,4-Benzenetricarboxylic acid, mixed decyl and octyl triesters	290-754-9	90218-76-1	90218761	-	-	4330														18%	-6.1	-6.4	-8.0
603-309-4	603-309-4	128973-77-3	128973773	-	-	4331														18%	-6.1	-6.4	-8.0

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Amines, C12-18-alkyl	268-953-7	68155-27-1	68155271	-	-	4332														18%	-6.1	-6.4	-8.0
Resin acids and Rosin acids, magnesium salts	270-461-2	68440-56-2	68440562	-	-	4333														18%	-6.1	-6.4	-8.0
619-079-3	619-079-3	949109-75-5	949109755	-	-	4334														18%	-6.1	-6.4	-8.0
orthoboric acid, compound with 2-aminoethanol	247-421-8	26038-87-9	26038879	-	-	4335														18%	-6.1	-6.4	-8.0
Fatty acids, C14-18 and C16-18-unsatd., zinc salts	266-936-9	67701-12-6	67701126	-	-	4336														18%	-6.1	-6.4	-8.0
Glycerides, tall-oil mono-, di-, and tri-	307-751-6	97722-02-6	97722026	-	-	4337														18%	-6.1	-6.4	-8.0
Dodecene, hydroformylation products, low-boiling	271-240-3	68526-92-1	68526921	-	-	4338														18%	-6.1	-6.4	-8.1
tetrahydromethylphthalic anhydride	234-290-7	11070-44-3	11070443	-	-	4339														18%	-6.1	-6.4	-8.1
Saccharomyces cerevisiae, ext.	283-294-5	84604-16-0	84604160	-	-	4340														18%	-6.1	-6.4	-8.1
Benzene, (1-methylethyl)-, oxidized, cumene residues, acetoph	309-849-4	101316-44-3	101316443	-	-	4341														18%	-6.1	-6.4	-8.1
Distillates (petroleum), heavy steam-cracked	309-939-3	101631-14-5	101631145	-	-	4342														18%	-6.1	-6.4	-8.1
2,6-dimethylmorpholine	205-509-3	141-91-3	141913	-	-	4343														18%	-6.1	-6.4	-8.1
Glycerides, C14-18	266-945-8	67701-27-3	67701273	-	-	4344														18%	-6.1	-6.4	-8.1
Hydrocarbons, C4-10-unsatd.	271-040-6	68514-38-5	68514385	-	-	4345														18%	-6.1	-6.4	-8.1
Alkenes, C6-	271-208-9	68526-52-3	68526523	-	-	4346														18%	-6.1	-6.4	-8.1
Alkenes, C10-12, C11-rich	271-214-1	68526-57-8	68526578	-	-	4347														18%	-6.1	-6.4	-8.1
Alkenes, C6-10, hydroformylation products, high-boiling	271-230-9	68526-82-9	68526829	-	-	4348														18%	-6.1	-6.4	-8.1
1-Propene, hydroformylation products, high-boiling	271-363-2	68551-11-1	68551111	-	-	4349														18%	-6.1	-6.4	-8.1
Hydrocarbons, C4 and C8, butene concentrator by-product	271-739-6	68606-29-1	68606291	-	-	4350														18%	-6.1	-6.4	-8.1
Disilane, chloro Me derivs.	273-054-8	68937-17-7	68937177	-	-	4351														18%	-6.1	-6.4	-8.1
1,2-Benzenedicarboxylic acid, di-C1-13 alkyl esters, manuf. of, b	284-310-3	84852-02-8	84852028	-	-	4352														18%	-6.1	-6.4	-8.1
Alkyl iodides, C8-14, γ-ω-perfluoro	289-100-5	85995-91-1	85995911	-	-	4353														18%	-6.1	-6.4	-8.1
Naphtha (coal), distn. residues	292-636-2	90641-12-6	90641126	-	-	4354														18%	-6.1	-6.4	-8.1
anthracene oil, anthracene paste, distn. lights	295-278-5	91995-17-4	91995174	-	-	4355														18%	-6.1	-6.4	-8.1
Alkenes, C11-14	297-794-6	93762-77-7	93762777	-	-	4356														18%	-6.1	-6.4	-8.1
Alkenes, C6-8-branched, C7-rich	307-298-4	97592-99-9	97592999	-	-	4357														18%	-6.1	-6.4	-8.1
bis(isopropyl)naphthalene	254-052-6	38640-62-9	38640629	-	-	4358														18%	-6.1	-6.4	-8.1
Propylidynetrimethanol, ethoxylated	500-110-3	50586-59-9	50586599	-	-	4359														18%	-6.1	-6.4	-8.1
Terpineol	232-268-1	8000-41-7	8000417	-	-	4360														18%	-6.1	-6.4	-8.1
oxydipropyl dibenzoate	248-258-5	27138-31-4	27138314	-	-	4361														18%	-6.1	-6.4	-8.1
Paraffin oils, sulfochlorinated, saponified	269-144-1	68188-18-1	68188181	-	-	4362														18%	-6.1	-6.4	-8.1
601-601-6	601-601-6	119345-04-9	119345049	-	-	4363														18%	-6.1	-6.4	-8.1
603-094-7	603-094-7	125904-11-2	125904112	-	-	4364														18%	-6.1	-6.4	-8.1
methyl 3-oxo-2-pentylcyclopentaneacetate	246-495-9	24851-98-7	24851987	-	-	4365														18%	-6.1	-6.4	-8.1
4,4'-methylenebis(cyclohexylamine)	217-168-8	1761-71-3	1761713	-	-	4366														18%	-6.1	-6.4	-8.1
diisononyl adipate	251-646-7	33703-08-1	33703081	-	-	4367														18%	-6.1	-6.4	-8.1
Rosin, reaction products with formaldehyde	293-659-0	91081-53-7	91081537	-	-	4368														18%	-6.1	-6.4	-8.1
ditolyl ether	248-948-6	28299-41-4	28299414	-	-	4369														18%	-6.1	-6.4	-8.1
627-034-4	627-034-4	1213789-63-9	1213789639	-	-	4370														18%	-6.1	-6.4	-8.1
Amides, coco, N-[3-(dimethylamino)propyl]	268-771-8	68140-01-2	68140012	-	-	4371														18%	-6.1	-6.4	-8.1
Linseed oil, oxidized	272-038-8	68649-95-6	68649956	-	-	4372														18%	-6.1	-6.4	-8.1
Fatty acids, C5-10, esters with pentaerythritol	270-291-9	68424-31-7	68424317	-	-	4373														18%	-6.1	-6.4	-8.1
Phenol, 4-methyl-, reaction products with dicyclopentadiene ar	271-867-2	68610-51-5	68610515	-	-	4374														18%	-6.2	-6.5	-8.1
hexadecene	248-131-4	26952-14-7	26952147	-	-	4375														18%	-6.2	-6.5	-8.1
2,2'-Oxydiethanol, propoxylated	500-031-4	9051-51-8	9051518	-	-	4376														18%	-6.2	-6.5	-8.1
Benzenesulfonic acid, mono-C10-13-alkyl derivs., compds. with	287-335-8	85480-55-3	85480553	-	-	4377														18%	-6.2	-6.5	-8.1
Fatty acids, C16-18, C16-18-alkyl esters	306-797-4	97404-33-6	97404336	-	-	4378														18%	-6.2	-6.5	-8.1
1,6-bis(2,3-epoxypropoxy)hexane	240-260-4	16096-31-4	16096314	-	-	4379														18%	-6.2	-6.5	-8.1
Alcohols, C9-11-branched	271-360-6	68551-08-6	68551086	-	-	4380														18%	-6.2	-6.5	-8.1
Rosin, hydrogenated	266-041-3	65997-06-0	65997060	-	-	4381														18%	-6.2	-6.5	-8.1
Protein hydrolyzates, animal	309-203-1	100085-61-8	100085618	-	-	4382														18%	-6.2	-6.5	-8.1
Dec-1-ene, dimers, hydrogenated	500-228-5	68649-11-6	68649116	-	-	4383														18%	-6.2	-6.5	-8.1
4,4'-Methylenediphenyl diisocyanate, oligomeric reaction prod	500-262-0	75880-28-3	75880283	-	-	4384														18%	-6.2	-6.5	-8.1
642-362-8	642-362-8	1190630-03-5	1190630035	-	-	4385														18%	-6.2	-6.5	-8.1
diundecyl phthalate, branched and linear	287-401-6	85507-79-5	85507795	-	-	4386														18%	-6.2	-6.5	-8.2
oxybis(methyl-2,1-ethanediyl) diacrylate	260-754-3	57472-68-1	57472681	-	-	4387														18%	-6.2	-6.5	-8.2
diisotridecyl adipate	247-660-8	26401-35-4	26401354	-	-	4388														18%	-6.2	-6.5	-8.2
polychloro copper phthalocyanine	215-524-7	1328-53-6	1328536	-	-	4389														18%	-6.2	-6.5	-8.2
Benzene, (1-methylethyl)-, distn. residues	273-050-6	68936-98-1	68936981	-	-	4390														18%	-6.2	-6.5	-8.2
1,2-Benzenedicarboxylic acid, di-C16-18-alkyl esters	290-580-3	90193-76-3	90193763	-	-	4391														18%	-6.2	-6.5	-8.2
Resin acids and Rosin acids, esters with triethylene glycol	232-478-3	8050-25-7	8050257	-	-	4392														18%	-6.2	-6.5	-8.2
1,2-Benzenedicarboxylic acid, di-C11-14-branched alkyl esters,	271-089-3	68515-47-9	68515479	-	-	4393														18%	-6.2	-6.5	-8.2
628-856-6	628-856-6	1218787-29-1	1218787291	-	-	4394														18%	-6.2	-6.5	-8.2
Decanoic acid, ester with 2-ethyl-2-(hydroxymethyl)-1,3-propar	234-392-1	11138-60-6	11138606	-	-	4395														18%	-6.2	-6.5	-8.2
Alcohols, C6-24, distn. residues	310-080-1	102242-49-9	102242499	-	-	4396														18%	-6.2	-6.5	-8.2
604-767-8	604-767-8	151006-60-9	151006609	-	-	4397														18%	-6.2	-6.5	-8.2
Fatty acids, C16-18 and C18-unsatd., Me esters, distn. residues	271-692-1	68604-41-1	68604411	-	-	4398														18%	-6.2	-6.6	-8.2
Phosphorodithioic acid, mixed O,O-bis(1,3-dimethylbutyl and is	283-392-8	84605-29-8	84605298	-	-	4399														18%	-6.3	-6.6	-8.2
dibenzyltoluene	248-097-0	26898-17-9	26898179	-	-	4400														18%	-6.3	-6.6	-8.2
Phosphorodithioic acid, mixed O,O-bis(sec-Bu and 1,3-dimethy	272-238-5	68784-31-6	68784316	-	-	4401														18%	-6.3	-6.6	-8.2
Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu	288-917-4	85940-28-9	85940289	-	-	4402														18%	-6.3	-6.6	-8.2
Oils, fish, oxidized	269-122-1	68187-75-7	68187757	-	-	4403														18%	-6.3	-6.6	-8.2
Oxirane, mono[(C12-14-alkyloxy)methyl] derivs.	271-846-8	68609-97-2	68609972	-	-	4404														18%	-6.3	-6.6	-8.2
diundecyl phthalate	222-884-9	3648-20-2	3648202	-	-	4405														18%	-6.3	-6.6	-8.2
isooctyl acrylate	249-707-8	29590-42-9	29590429	-	-	4406														18%	-6.3	-6.6	-8.2

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylindeno[5,6-c]pyra	214-946-9	1222-05-5	1222055	-	-	4407														18%	-6.3	-6.6	-8.2
Fatty acids, hydrogenated tallow, distn. residues	274-307-5	70084-85-4	70084854	-	-	4408														18%	-6.3	-6.6	-8.2
ethanol, 2-methoxy-, manufacture of, by-products from	310-289-8	161907-79-5	161907795	-	-	4409														18%	-6.3	-6.6	-8.2
Heptanoic acid, mixed esters with pentaerythritol and valeric a	270-474-3	68441-94-1	68441941	-	-	4410														18%	-6.3	-6.6	-8.2
Fatty acids, tall-oil, oligomeric reaction products with maleic an	500-451-8	160901-14-4	160901144	-	-	4411														18%	-6.3	-6.6	-8.2
Cashew, nutshell liq.	232-355-4	8007-24-7	8007247	-	-	4412														18%	-6.3	-6.6	-8.3
zinc bis[O,O-bis(2-ethylhexyl)] bis(dithiophosphate)	224-235-5	4259-15-8	4259158	-	-	4413														18%	-6.3	-6.6	-8.3
Quaternary ammonium compounds, di-C16-18-alkyldimethyl, c	295-835-2	92129-33-4	92129334	-	-	4414														18%	-6.3	-6.6	-8.3
Alcohols, C16-18 and C18-unsatd., ethoxylated	500-236-9	68920-66-1	68920661	-	-	4415														18%	-6.3	-6.6	-8.3
Oils, vegetable, sulfonated, sodium salts	307-044-2	97489-04-8	97489048	-	-	4416														18%	-6.3	-6.6	-8.3
DL-menthol	216-074-4	1490-04-6	1490046	-	-	4417														18%	-6.3	-6.6	-8.3
Alkanes, C16-20-iso-	292-461-1	90622-59-6	90622596	-	-	4418														18%	-6.3	-6.6	-8.3
Extract residues (coal), naphthalene oil alk., distn. residues	292-628-9	90641-05-7	90641057	-	-	4419														18%	-6.3	-6.6	-8.3
Extract residues (coal), benzole fraction acid	298-725-2	93821-38-6	93821386	-	-	4420														18%	-6.3	-6.6	-8.3
Humic acids, potassium salts	271-030-1	68514-28-3	68514283	-	-	4421														18%	-6.3	-6.6	-8.3
octadecene	248-205-6	27070-58-2	27070582	-	-	4422														18%	-6.3	-6.6	-8.3
xylenesulphonic acid	246-839-8	25321-41-9	25321419	-	-	4423														18%	-6.3	-6.6	-8.3
1,2-Benzenedicarboxylic acid, di-C9-11-branched and linear alk	271-085-1	68515-43-5	68515435	-	-	4424														18%	-6.3	-6.6	-8.3
Fatty acids, C16-18 and C18-unsatd., 2-ethylhexyl esters	285-207-6	85049-37-2	85049372	-	-	4425														18%	-6.3	-6.6	-8.3
Sulfuric acid, mono-C12-16-alkyl esters, sodium salts	277-362-3	73296-89-6	73296896	-	-	4426														18%	-6.3	-6.6	-8.3
615-276-3	615-276-3	71302-83-5	71302835	-	-	4427														18%	-6.3	-6.6	-8.3
potassium methylsilanetriolate	250-807-9	31795-24-1	31795241	-	-	4428														18%	-6.3	-6.6	-8.3
Resin acids and Rosin acids, hydrogenated, esters with glycerol	266-042-9	65997-13-9	65997139	-	-	4429														18%	-6.3	-6.7	-8.3
Distillates (coal tar), naphthalene oil crystn. mother liquor	295-310-8	91995-49-2	91995492	-	-	4430														18%	-6.4	-6.7	-8.3
Alkenes, C7-9, hydroformylation products, distn. residues, heav	308-482-7	98072-31-2	98072312	-	-	4431														18%	-6.4	-6.7	-8.3
Alcohols, C9-11-branched and linear	288-284-4	85711-26-8	85711268	-	-	4432														18%	-6.4	-6.7	-8.3
Fatty acids, C16-18, 2-ethylhexyl esters	292-951-5	91031-48-0	91031480	-	-	4433														18%	-6.4	-6.7	-8.3
tetraphenyl m-phenylene bis(phosphate)	260-830-6	57583-54-7	57583547	-	-	4434														18%	-6.4	-6.7	-8.3
1-Hexanol, 2-ethyl-, manuf. of, by-products from, distn. residue	271-832-1	68609-68-7	68609687	-	-	4435														18%	-6.4	-6.7	-8.3
Tar acids, methylphenol fraction	284-892-9	84989-04-8	84989048	-	-	4436														18%	-6.4	-6.7	-8.3
629-715-1	629-715-1	1226892-43-8	1226892438	-	-	4437														18%	-6.4	-6.7	-8.3
2,2'-dimethyl-4,4'-methylenebis(cyclohexylamine)	229-962-1	6864-37-5	6864375	-	-	4438														18%	-6.4	-6.7	-8.4
Fatty acids, C8-16	287-973-7	85631-26-1	85631261	-	-	4439														18%	-6.4	-6.7	-8.4
Ethanol, 2-amino-, reaction products with ammonia, by-produc	272-729-4	68910-05-4	68910054	-	-	4440														18%	-6.4	-6.7	-8.4
629-721-4	629-721-4	308062-60-4	308062604	-	-	4441														18%	-6.4	-6.7	-8.4
1,4-Benzenediamine, N,N'-mixed Ph and tolyl derivs.	273-227-8	68953-84-4	68953844	-	-	4442														18%	-6.4	-6.7	-8.4
Reaction mass of 6-O-alfa-D-glucopyranosyl-D-fructofuranose a	700-515-7	1236007-63-8	1236007638	-	-	4443														18%	-6.4	-6.7	-8.4
Benzoic acid, C12-15-alkyl esters	270-112-4	68411-27-8	68411278	-	-	4444														18%	-6.4	-6.7	-8.4
sodium xylenesulphonate	215-090-9	1300-72-7	1300727	-	-	4445														18%	-6.4	-6.7	-8.4
terphenyl	247-477-3	26140-60-3	26140603	-	-	4446														18%	-6.5	-6.8	-8.4
cresol	215-293-2	1319-77-3	1319773	-	-	4447														18%	-6.5	-6.8	-8.4
Terphenyl, hydrogenated	262-967-7	61788-32-7	61788327	-	-	4448														18%	-6.5	-6.8	-8.4
1,4-bis(2,3-epoxypropoxy)butane	219-371-7	2425-79-8	2425798	-	-	4449														18%	-6.5	-6.8	-8.4
dichloromethylbenzene	249-854-8	29797-40-8	29797408	-	-	4450														18%	-6.5	-6.8	-8.4
617-779-3	617-779-3	85940-94-9	85940949	-	-	4451														18%	-6.5	-6.8	-8.4
Glycerides, C12-18	266-944-2	67701-26-2	67701262	-	-	4452														18%	-6.5	-6.8	-8.4
629-719-3	629-719-3	1219010-04-4	1219010044	-	-	4453														18%	-6.5	-6.8	-8.4
Fatty acids, C5-9, esters with pentaerythritol	270-290-3	68424-30-6	68424306	-	-	4454														18%	-6.5	-6.8	-8.4
601-238-3	601-238-3	113163-37-4	113163374	-	-	4455														18%	-6.5	-6.8	-8.5
4,4'-Methylenediphenyl diisocyanate, oligomeric reaction prod	500-312-1	123714-19-2	123714192	-	-	4456														18%	-6.5	-6.8	-8.5
acrylic acid, monoester with propane-1,2-diol	247-118-0	25584-83-2	25584832	-	-	4457														18%	-6.5	-6.8	-8.5
604-580-1	604-580-1	147256-33-5	147256335	-	-	4458														18%	-6.5	-6.8	-8.5
Dodecene, hydroformylation products, high-boiling	271-239-8	68526-91-0	68526910	-	-	4459														18%	-6.5	-6.8	-8.5
Glycerides, C16-18 and C18-unsatd., deodorizer distillates	272-911-3	68920-03-6	68920036	-	-	4460														18%	-6.5	-6.8	-8.5
Fatty acids, C16-18, sodium salts	270-299-2	68424-38-4	68424384	-	-	4461														18%	-6.5	-6.8	-8.5
Glycerides, C16-18 and C18-unsatd. mono-	294-571-5	91744-09-1	91744091	-	-	4462														18%	-6.5	-6.8	-8.5
Pentaerythritol, propoxylated	500-030-9	9051-49-4	9051494	-	-	4463														18%	-6.5	-6.8	-8.5
Glycerides, C16-18 and C18-unsatd. mono-, di and tri-	294-582-5	91744-20-6	91744206	-	-	4464														18%	-6.5	-6.8	-8.5
Subtilisin	232-752-2	9014-01-1	9014011	-	-	4465														18%	-6.5	-6.8	-8.5
stearic acid, monoester with glycerol	250-705-4	31566-31-1	31566311	-	-	4466														18%	-6.5	-6.8	-8.5
Quaternary ammonium compounds, C20-22-alkyltrimethyl, chl	271-756-9	68607-24-9	68607249	-	-	4467														18%	-6.5	-6.8	-8.5
diethylmethylbenzenediamine	270-877-4	68479-98-1	68479981	-	-	4468														18%	-6.5	-6.8	-8.5
Polysulfides, di-tert-dodecyl	270-335-7	68425-15-0	68425150	-	-	4469														18%	-6.5	-6.8	-8.5
Fatty acids, coco, 2-ethylhexyl esters	295-366-3	92044-87-6	92044876	-	-	4470														18%	-6.5	-6.8	-8.5
2,2',2''-Nitrilotriethanol, propoxylated	500-094-8	37208-53-0	37208530	-	-	4471														18%	-6.5	-6.8	-8.5
diethylbenzene	246-874-9	25340-17-4	25340174	-	-	4472														18%	-6.6	-6.9	-8.5
Distillates (coal tar), benzole fraction, BTX-rich	309-984-9	101896-26-8	101896268	-	-	4473														18%	-6.6	-6.9	-8.5
Solvent naphtha (coal)	266-013-0	65996-79-4	65996794	-	-	4474														18%	-6.6	-6.9	-8.5
1,3,5-triazine-2,4,6-triamine phosphate	255-449-7	41583-09-9	41583099	-	-	4475														18%	-6.6	-6.9	-8.5
Fatty acids, C14-22, 2-ethylhexyl esters, epoxidized	305-962-8	95370-96-0	95370960	-	-	4476														18%	-6.6	-6.9	-8.5
Rape oil, oxidized	305-871-3	95193-59-2	95193592	-	-	4477														18%	-6.6	-6.9	-8.5
4,4'-Isopropylidenediphenol, propoxylated	500-097-4	37353-75-6	37353756	-	-	4478														18%	-6.6	-6.9	-8.5
Alcohols, lanolin	232-430-1	8027-33-6	8027336	-	-	4479														18%	-6.6	-6.9	-8.5
phenol, 2,4-dinitro-, sulfurized, leuco derivatives	266-273-5	66241-11-0	66241110	-	-	4480														18%	-6.6	-6.9	-8.5
Fatty acids, lanolin	270-302-7	68424-43-1	68424431	-	-	4481														18%	-6.6	-6.9	-8.5

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
benzyltoluene	248-654-8	27776-01-8	27776018	-	-	4482														18%	-6.6	-6.9	-8.5
614-503-3	614-503-3	68441-62-3	68441623	-	-	4483														18%	-6.6	-6.9	-8.5
2,2,4(or 2,4,4)-trimethylhexane-1,6-diamine	247-063-2	25513-64-8	25513648	-	-	4484														18%	-6.6	-6.9	-8.5
Fatty acids, C16-18 and C18-unsatd., Bu esters	284-863-0	84988-74-9	84988749	-	-	4485														18%	-6.6	-6.9	-8.5
Fatty acids, C18-unsatd., dimers, 2-ethylhexyl esters	500-204-4	68334-05-4	68334054	-	-	4486														18%	-6.6	-6.9	-8.6
Rosin, fumarated, reaction products with glycerol and pentaery	296-047-1	92202-14-7	92202147	-	-	4487														18%	-6.6	-6.9	-8.6
Aromatic hydrocarbons, C9-12, benzene distn.	295-551-9	92062-36-7	92062367	-	-	4488														18%	-6.6	-6.9	-8.6
3,6,9,12-tetraazatetradecamethylenediamine	223-775-9	4067-16-7	4067167	-	-	4489														18%	-6.6	-6.9	-8.6
potassium trihydrogen dioxalate	204-874-6	127-96-8	127968	-	-	4490														18%	-6.6	-6.9	-8.6
Lecithins, acetylated	293-316-5	91053-50-8	91053508	-	-	4491														18%	-6.6	-6.9	-8.6
4,4'-Methylenediphenyl diisocyanate, oligomeric reaction prod	500-415-1	158885-29-1	158885291	-	-	4492														18%	-6.6	-6.9	-8.6
2-aminoethanol, monoester with boric acid	233-829-3	10377-81-8	10377818	-	-	4493														18%	-6.6	-6.9	-8.6
Phenol, styrenated	262-975-0	61788-44-1	61788441	-	-	4494														18%	-6.6	-6.9	-8.6
[1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[tert-butyl] p	246-678-3	25155-25-3	25155253	-	-	4495														18%	-6.6	-6.9	-8.6
Fatty acids, C12-20 and C12-20-unsatd., 2-ethylhexyl esters	292-811-3	91001-42-2	91001422	-	-	4496														18%	-6.6	-6.9	-8.6
Fatty acids, coco, triesters with trimethylolpropane	287-640-6	85566-29-6	85566296	-	-	4497														18%	-6.6	-7.0	-8.6
neodecanoyl chloride	254-875-0	40292-82-8	40292828	-	-	4498														18%	-6.6	-7.0	-8.6
Urea, reaction products with formaldehyde, glyoxal and metha	296-665-1	92908-36-6	92908366	-	-	4499														18%	-6.6	-7.0	-8.6
606-203-6	606-203-6	1902-01-8	1902018	-	-	4500														18%	-6.6	-7.0	-8.6
600-444-0	600-444-0	103513-05-9	103513059	-	-	4501														18%	-6.6	-7.0	-8.6
Fatty acids, C12-14	292-771-7	90990-10-6	90990106	-	-	4502														18%	-6.6	-7.0	-8.6
629-757-0	629-757-0	1224966-15-7	1224966157	-	-	4503														18%	-6.7	-7.0	-8.6
Benzenesulfonic acid, mono-C11-13-branched alkyl derivs.	271-807-5	68608-88-8	68608888	-	-	4504														18%	-6.7	-7.0	-8.6
Fusel oil	232-395-2	8013-75-0	8013750	-	-	4505														18%	-6.7	-7.0	-8.6
605-717-8	605-717-8	174333-80-3	174333803	-	-	4506														18%	-6.7	-7.0	-8.6
4,4'-Isopropylidenediphenol, ethoxylated	500-082-2	32492-61-8	32492618	-	-	4507														18%	-6.7	-7.0	-8.6
Alcohols, C7-9	266-417-7	66587-56-2	66587562	-	-	4508														18%	-6.7	-7.0	-8.6
benzyl 3-isobutyryloxy-1-isopropyl-2,2-dimethylpropyl phthalat	240-920-1	16883-83-3	16883833	-	-	4509														18%	-6.7	-7.0	-8.6
Alcohols, C12-13, ethoxylated	500-165-3	66455-14-9	66455149	-	-	4510														18%	-6.7	-7.0	-8.6
Fatty acids, C18-unsatd., dimers, hydrogenated	500-231-1	68783-41-5	68783415	-	-	4511														18%	-6.7	-7.0	-8.6
Hydrocarbons, C4, 1,3-butadiene-free, polymd., tetraisobutyler	297-628-2	93685-80-4	93685804	-	-	4512														18%	-6.7	-7.0	-8.6
Fatty acids, C16-18 and C18-unsatd., mixed esters with adipic a	292-832-8	91001-61-5	91001615	-	-	4513														18%	-6.7	-7.0	-8.6
Eucalyptus globulus, ext.	283-406-2	84625-32-1	84625321	-	-	4514														18%	-6.7	-7.0	-8.6
Amines, C12-18-alkyldimethyl	269-923-6	68391-04-8	68391048	-	-	4515														18%	-6.7	-7.0	-8.7
4,4'-Isopropylidenediphenol, oligomeric reaction products with	500-089-0	36425-15-7	36425157	-	-	4516														18%	-6.7	-7.0	-8.7
Fatty acids, C18-unsatd., trimers	500-239-5	68937-90-6	68937906	-	-	4517														18%	-6.7	-7.0	-8.7
Boric acid (H3BO3), reaction products with ethanolamine	302-207-4	94095-04-2	94095042	-	-	4518														18%	-6.7	-7.0	-8.7
Poly[oxy(methyl-1,2-ethanediyl)],α-butyl-ω-hydroxy-	500-003-1	9003-13-8	9003138	-	-	4519														18%	-6.7	-7.0	-8.7
Rosin, maleated	232-480-4	8050-28-0	8050280	-	-	4520														18%	-6.7	-7.0	-8.7
Fatty acids, sunflower-oil, conjugated	273-195-5	68953-27-5	68953275	-	-	4521														18%	-6.7	-7.0	-8.7
diisodecyl azelate	249-044-4	28472-97-1	28472971	-	-	4522														18%	-6.7	-7.0	-8.7
diisodecyl adipate	248-299-9	27178-16-1	27178161	-	-	4523														18%	-6.7	-7.0	-8.7
4,4'-Isopropylidenediphenol, oligomeric reaction products with	500-101-4	38294-64-3	38294643	-	-	4524														18%	-6.7	-7.0	-8.7
Nonylphenol, branched, ethoxylated	500-209-1	68412-54-4	68412544	-	-	4525														18%	-6.7	-7.0	-8.7
Soaps, stocks, vegetable-oil, acidulated	273-179-8	68952-95-4	68952954	-	-	4526														18%	-6.7	-7.0	-8.7
Ionone, methyl-	215-635-0	1335-46-2	1335462	-	-	4527														18%	-6.7	-7.0	-8.7
Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, cl	273-501-7	68987-63-3	68987633	-	-	4528														18%	-6.7	-7.0	-8.7
627-083-1	627-083-1	244235-47-0	244235470	-	-	4529														18%	-6.7	-7.0	-8.7
Resin acids and Rosin acids, calcium zinc salts	269-825-3	68334-35-0	68334350	-	-	4530														18%	-6.7	-7.0	-8.7
Fatty acids, C14-18 and C16-18-unsatd., barium salts	305-998-4	95465-85-3	95465853	-	-	4531														18%	-6.7	-7.0	-8.7
Alkenes, C11-12, hydroformylation products, distn. residues	292-427-6	90622-27-8	90622278	-	-	4532														18%	-6.7	-7.0	-8.7
Ethanol, 2,2'-oxybis-, reaction products with ammonia, morphc	272-712-1	68909-77-3	68909773	-	-	4533														18%	-6.7	-7.0	-8.7
Phenol, isobutylenated, phosphate (3:1)	273-065-8	68937-40-6	68937406	-	-	4534														18%	-6.7	-7.1	-8.7
tris(methylphenyl) phosphate	215-548-8	1330-78-5	1330785	-	-	4535														18%	-6.7	-7.1	-8.7
Fatty acids, C18-unsatd., dimers, oligomeric reaction products	500-191-5	68082-29-1	68082291	-	-	4536														18%	-6.8	-7.1	-8.7
tricyclodecanedimethanol	248-096-5	26896-48-0	26896480	-	-	4537														18%	-6.8	-7.1	-8.7
Quaternary ammonium compounds, di-C12-18-alkyldimethyl, c	269-924-1	68391-05-9	68391059	-	-	4538														18%	-6.8	-7.1	-8.7
Fatty acids, C16-22	268-103-5	68002-88-0	68002880	-	-	4539														18%	-6.8	-7.1	-8.7
Oils, animal, sulfated, sodium salts	304-835-4	94279-90-0	94279900	-	-	4540														18%	-6.8	-7.1	-8.7
Oils, vegetable, sulfated	263-113-6	61790-19-0	61790190	-	-	4541														18%	-6.8	-7.1	-8.7
Octadecanoic acid, branched and linear	269-214-1	68201-37-6	68201376	-	-	4542														18%	-6.8	-7.1	-8.7
Decanoic acid, mixed esters with dipentaerythritol, octanoic ac	270-470-1	68441-66-7	68441667	-	-	4543														18%	-6.8	-7.1	-8.7
614-114-9	614-114-9	67746-08-1	67746081	-	-	4544														18%	-6.8	-7.1	-8.8
Glycerides, C16-22	268-083-8	68002-70-0	68002700	-	-	4545														18%	-6.8	-7.1	-8.8
629-725-6	629-725-6	1226892-45-0	1226892450	-	-	4546														18%	-6.8	-7.1	-8.8
Reaction mass of ethyl (2S,3S)-3,4-dibromo-2-methylbutanoate	700-225-0	1160806-44-9	1160806449	-	-	4547														18%	-6.8	-7.1	-8.8
605-322-0	605-322-0	163292-61-3	163292613	-	-	4548														18%	-6.8	-7.1	-8.8
1-hydroxy-2-methylpentan-3-one	939-893-5	27970-79-2	27970792	-	-	4549														18%	-6.8	-7.1	-8.8
1,4-anhydro-2,5-dideoxy-2-(methoxycarbonyl)-1-thiopent-3-ul	619-801-7	66319-07-1	66319071	-	-	4550														18%	-6.8	-7.1	-8.8
Benzene, butyl-, branched and linear	270-126-0	68411-44-9	68411449	-	-	4551														18%	-6.8	-7.1	-8.8
Benzenesulfonic acid, mono-C11-13-branched alkyl derivs., calc	273-234-6	68953-96-8	68953968	-	-	4552														18%	-6.8	-7.1	-8.8
Fatty acids, C16-18, C12-18-alkyl esters	306-083-2	95912-87-1	95912871	-	-	4553														18%	-6.8	-7.1	-8.8
Fatty acids, C16-18, isotridecyl esters	306-084-8	95912-88-2	95912882	-	-	4554														18%	-6.8	-7.1	-8.8
629-705-7	629-705-7	1228186-15-9	1228186159	-	-	4555														18%	-6.8	-7.1	-8.8
Cinnamomum zeylanicum, ext.	283-479-0	84649-98-9	84649989	-	-	4556														18%	-6.8	-7.1	-8.8

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
629-850-6	629-850-6	1245638-61-2	1245638612	-	-	4557														18%	-6.8	-7.1	-8.8
sorbitan laurate	215-663-3	1338-39-2	1338392	-	-	4558														18%	-6.8	-7.1	-8.8
Tar acids, xylenol fraction	284-895-5	84989-06-0	84989060	-	-	4559														18%	-6.8	-7.1	-8.8
triisotridecyl phosphite	278-758-9	77745-66-5	77745665	-	-	4560														18%	-6.8	-7.1	-8.8
Ethanol, 2,2'-iminobis-, N-(C13-15-branched and linear alkyl) de	308-208-6	97925-95-6	97925956	-	-	4561														18%	-6.8	-7.1	-8.8
diisotridecyl phthalate	248-368-3	27253-26-5	27253265	-	-	4562														18%	-6.8	-7.1	-8.8
methyl-1H-benzotriazole	249-596-6	29385-43-1	29385431	-	-	4563														18%	-6.8	-7.1	-8.8
diisodecyl phenyl phosphite	247-098-3	25550-98-5	25550985	-	-	4564														18%	-6.8	-7.1	-8.8
dihydro-3-(tetrapropenyl)furan-2,5-dione	247-781-6	26544-38-7	26544387	-	-	4565														18%	-6.8	-7.1	-8.8
2,4,7,9-tetramethyldec-5-yne-4,7-diol	204-809-1	126-86-3	126863	-	-	4566														18%	-6.8	-7.1	-8.8
Castor oil, sulfated, sodium salt	269-123-7	68187-76-8	68187768	-	-	4567														18%	-6.8	-7.1	-8.8
2,2'-(C16-18 (evennumbered, C18 unsaturated) alkyl imino) die	620-540-6	1218787-32-6	1218787326	-	-	4568														18%	-6.8	-7.2	-8.8
Phosphorodithioic acid, mixed O,O-bis(iso-Bu and pentyl) ester	270-608-0	68457-79-4	68457794	-	-	4569														18%	-6.8	-7.2	-8.8
4-tert-butylcyclohexyl acetate	250-954-9	32210-23-4	32210234	-	-	4570														18%	-6.8	-7.2	-8.8
Acetic acid, chloro-, sodium salt, reaction products with 4,5-dih	271-794-6	68608-66-2	68608662	-	-	4571														18%	-6.8	-7.2	-8.8
hexahydromethylphthalic anhydride	247-094-1	25550-51-0	25550510	-	-	4572														18%	-6.9	-7.2	-8.8
614-668-1	614-668-1	68610-97-9	68610979	-	-	4573														18%	-6.9	-7.2	-8.8
Decanoic acid, mixed diesters with octanoic acid and propylene	271-516-3	68583-51-7	68583517	-	-	4574														18%	-6.9	-7.2	-8.8
1-Butene, chlorinated, epoxidized, distn. residues	304-781-1	94279-37-5	94279375	-	-	4575														18%	-6.9	-7.2	-8.8
sorbitan stearate	215-664-9	1338-41-6	1338416	-	-	4576														18%	-6.9	-7.2	-8.8
Amylase, gluco-	232-877-2	9032-08-0	9032080	-	-	4577														18%	-6.9	-7.2	-8.8
641-136-6	641-136-6	1160164-88-4	1160164884	-	-	4578														18%	-6.9	-7.2	-8.8
Amines, di-C12-18-alkylmethyl	270-418-8	68439-75-8	68439758	-	-	4579														18%	-6.9	-7.2	-8.8
Phenol, dodecyl-, sulfurized, calcium salts	272-486-4	68855-45-8	68855458	-	-	4580														18%	-6.9	-7.2	-8.8
extract residues (coal tar), high-temperature, naphthalene oil a	310-256-8	140362-65-8	140362658	-	-	4581														18%	-6.9	-7.2	-8.8
Amylase, α-	232-565-6	9000-90-2	9000902	-	-	4582														18%	-6.9	-7.2	-8.8
Ethanol, 2,2'-iminobis-, N-C12-18-alkyl derivs.	276-014-8	71786-60-2	71786602	-	-	4583														18%	-6.9	-7.2	-8.8
Fatty acids, tall-oil, Bu esters	267-028-5	67762-63-4	67762634	-	-	4584														18%	-6.9	-7.2	-8.8
605-318-9	605-318-9	163206-31-3	163206313	-	-	4585														18%	-6.9	-7.2	-8.8
Resin acids and Rosin acids, maleated, sodium salts	269-228-8	68201-60-5	68201605	-	-	4586														18%	-6.9	-7.2	-8.8
Oils, animal, sulfonated, sodium salts	305-979-0	95371-11-2	95371112	-	-	4587														18%	-6.9	-7.2	-8.9
4,4'-Methylenediphenyl diisocyanate, oligomeric reaction prod	500-439-2	159168-82-8	159168828	-	-	4588														18%	-6.9	-7.2	-8.9
2-Propenenitrile, reaction products with ethylenediamine, hydr	272-727-3	68909-99-9	68909999	-	-	4589														18%	-6.9	-7.2	-8.9
tridecylamine, branched and linear	289-185-9	86089-17-0	86089170	-	-	4590														18%	-6.9	-7.2	-8.9
3-[C13-(branched)-alkyloxy]propionitrile	700-399-8	947522-81-8	947522818	-	-	4591														18%	-6.9	-7.2	-8.9
Nitriles, C16-18	268-079-6	68002-65-3	68002653	-	-	4592														18%	-6.9	-7.2	-8.9
Linseed oil, epoxidized	232-401-3	8016-11-3	8016113	-	-	4593														18%	-6.9	-7.2	-8.9
Rosin, oligomers	500-163-2	65997-05-9	65997059	-	-	4594														18%	-6.9	-7.2	-8.9
Alkanes, C10-13, chloro	287-476-5	85535-84-8	85535848	-	-	4595														18%	-6.9	-7.2	-8.9
2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl 3,4,5,6-tetrabromo	243-885-0	20566-35-2	20566352	-	-	4596														18%	-6.9	-7.2	-8.9
630-399-2	630-399-2	130169-56-1	130169561	-	-	4597														18%	-6.9	-7.2	-8.9
614-264-5	614-264-5	68081-77-6	68081776	-	-	4598														18%	-6.9	-7.2	-8.9
Fatty acids, C14-22	270-298-7	68424-37-3	68424373	-	-	4599														18%	-6.9	-7.2	-8.9
Glycerides, C8-18 and C18-unsatd. mono- and di-, acetates	293-170-2	91052-13-0	91052130	-	-	4600														18%	-6.9	-7.2	-8.9
Octadecan-1-ol, ethoxylated	500-017-8	9005-00-9	9005009	-	-	4601														18%	-6.9	-7.2	-8.9
Fatty acids, C8-18 and C18-unsatd., esters with neopentyl glyco	286-072-6	85186-86-3	85186863	-	-	4602														18%	-6.9	-7.2	-8.9
Fatty acids, palm-oil, hydrogenated	282-486-6	84238-17-5	84238175	-	-	4603														18%	-6.9	-7.2	-8.9
Amines, N-C12-18-alkyltrimethylenedi-	268-957-9	68155-37-3	68155373	-	-	4604														18%	-6.9	-7.2	-8.9
Tar, wood	294-436-0	91722-33-7	91722337	-	-	4605														18%	-6.9	-7.2	-8.9
N-(2-hydroxyethyl)stearamide	203-883-2	111-57-9	111579	-	-	4606														18%	-6.9	-7.2	-8.9
603-894-6	603-894-6	135108-88-2	135108882	-	-	4607														18%	-6.9	-7.2	-8.9
Benzenesulfonic acid, propenated, calcium salt, overbased	271-877-7	68610-84-4	68610844	-	-	4608														18%	-6.9	-7.3	-8.9
trixylyl phosphate	246-677-8	25155-23-1	25155231	-	-	4609														18%	-6.9	-7.3	-8.9
Ethanol, 2-amino-, reaction products with ammonia, 1-piperazi	296-543-8	92731-41-4	92731414	-	-	4610														18%	-7.0	-7.3	-8.9
Alkenes, C13-14, hydroformylation products, distn. residues	292-429-7	90622-29-0	90622290	-	-	4611														18%	-7.0	-7.3	-8.9
Hexanoic acid, 2-ethyl-, C16-18-alkyl esters	291-445-1	90411-68-0	90411680	-	-	4612														18%	-7.0	-7.3	-8.9
Gases (petroleum), extractive, C3-5, butene-isobutylene-rich	270-732-5	68477-42-9	68477429	-	-	4613														18%	-7.0	-7.3	-8.9
Pentaerythritol, ethoxylated, esters with acrylic acid	500-111-9	51728-26-8	51728268	-	-	4614														18%	-7.0	-7.3	-8.9
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate, oligo	500-287-7	103170-26-9	103170269	-	-	4615														18%	-7.0	-7.3	-8.9
dodecyl oleate	252-862-4	36078-10-1	36078101	-	-	4616														18%	-7.0	-7.3	-8.9
Toluene diisocyanate, oligomeric reaction products with water	500-299-2	110839-12-8	110839128	-	-	4617														18%	-7.0	-7.3	-8.9
603-931-6	603-931-6	135800-37-2	135800372	-	-	4618														18%	-7.0	-7.3	-8.9
Acid chlorides, coco	269-133-1	68187-89-3	68187893	-	-	4619														18%	-7.0	-7.3	-8.9
ethanol, 2-methoxy-, manufacture of, by-products from, esters	310-290-3	161907-80-8	161907808	-	-	4620														18%	-7.0	-7.3	-8.9
Acetic acid, oxo-, sodium salt, reaction products with ethylenec	283-042-4	84539-54-8	84539548	-	-	4621														18%	-7.0	-7.3	-8.9
Fatty acids, C16-18 and C18-unsatd., tetraesters with pentaeryt	271-694-2	68604-44-4	68604444	-	-	4622														18%	-7.0	-7.3	-8.9
Urea, reaction products with formaldehyde and glyoxal	296-664-6	92908-35-5	92908355	-	-	4623														18%	-7.0	-7.3	-8.9
zinc O,O,O',O'-tetrakis(1,3-dimethylbutyl) bis(phosphorodithioa	218-679-9	2215-35-2	2215352	-	-	4624														18%	-7.0	-7.3	-8.9
Propylidynetrimethanol, propoxylated, reaction products with	500-105-6	39423-51-3	39423513	-	-	4625														18%	-7.0	-7.3	-8.9
694-876-7	694-876-7	1345668-41-8	1345668418	-	-	4626														18%	-7.0	-7.3	-8.9
620-539-0	620-539-0	1218787-30-4	1218787304	-	-	4627														18%	-7.0	-7.3	-8.9
Glycerides, palm-oil mono-, hydrogenated, acetates	297-462-0	93572-32-8	93572328	-	-	4628														18%	-7.0	-7.3	-9.0
601-101-8	601-101-8	111497-86-0	111497860	-	-	4629														18%	-7.0	-7.3	-9.0
Tetrakis(hydroxymethyl)phosphonium chloride, oligomeric rea	500-057-6	27104-30-9	27104309	-	-	4630														18%	-7.0	-7.3	-9.0
Fatty acids, C5-10, esters with dipentaerythritol	275-093-6	70983-72-1	70983721	-	-	4631														18%	-7.0	-7.3	-9.0

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Cocoa, ext.	283-480-6	84649-99-0	84649990	-	-	4632														18%	-7.0	-7.3	-9.0
3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-indenyl propionate	272-805-7	68912-13-0	68912130	-	-	4633														18%	-7.0	-7.3	-9.0
hexyl D-glucoside	259-217-6	54549-24-5	54549245	-	-	4634														18%	-7.0	-7.3	-9.0
696-026-0	696-026-0	1395383-69-3	1395383693	-	-	4635														18%	-7.0	-7.3	-9.0
Fatty acids, coco, 2-sulfoethyl esters, sodium salts	263-052-5	61789-32-0	61789320	-	-	4636														18%	-7.0	-7.3	-9.0
Fatty acids, C8-18 and C18-unsatd., esters with trimethylolprop	286-075-2	85186-89-6	85186896	-	-	4637														18%	-7.0	-7.3	-9.0
zinc bis(O,O-diisooctyl) bis(dithiophosphate)	249-109-7	28629-66-5	28629665	-	-	4638														18%	-7.0	-7.3	-9.0
diisooctyl adipate	215-553-5	1330-86-5	1330865	-	-	4639														18%	-7.0	-7.3	-9.0
Glycerol, ethoxylated	500-075-4	31694-55-0	31694550	-	-	4640														18%	-7.0	-7.3	-9.0
Benzenamine, reaction products with aniline hydrochloride and	309-912-6	101357-15-7	101357157	-	-	4641														18%	-7.0	-7.3	-9.0
benzenesulfonic acid, 2,2'-(1,2-ethenediyl)bis[5-nitro-, disodiur	215-397-8	1325-54-8	1325548	-	-	4642														18%	-7.0	-7.4	-9.0
800-353-8	800-353-8	1379524-06-7	1379524067	-	-	4643														18%	-7.0	-7.4	-9.0
603-046-5	603-046-5	125301-84-0	125301840	-	-	4644														18%	-7.0	-7.4	-9.0
Decanoic acid, mixed esters with heptanoic acid, octanoic acid	268-596-7	68130-53-0	68130530	-	-	4645														18%	-7.0	-7.4	-9.0
Glycerol, ethoxylated, esters with acrylic acid	500-322-6	144086-03-3	144086033	-	-	4646														18%	-7.1	-7.4	-9.0
Propanenitrile, 3-amino-, N-tallow alkyl derivs.	272-268-9	68784-70-3	68784703	-	-	4647														18%	-7.1	-7.4	-9.0
sorbitan palmitate	247-568-8	26266-57-9	26266579	-	-	4648														18%	-7.1	-7.4	-9.0
ε-Caprolactone, oligomeric reaction products with propylidyne	500-099-5	37625-56-2	37625562	-	-	4649														18%	-7.1	-7.4	-9.0
bis(4-tert-butylcyclohexyl) peroxydicarbonate	239-557-1	15520-11-3	15520113	-	-	4650														18%	-7.1	-7.4	-9.0
614-283-9	614-283-9	68127-59-3	68127593	-	-	4651														18%	-7.1	-7.4	-9.0
4,4'-Isopropylidenedicyclohexanol, oligomeric reaction product	500-070-7	30583-72-3	30583723	-	-	4652														18%	-7.1	-7.4	-9.0
Resin acids and Rosin acids, hydrogenated, esters with pentaer	264-848-5	64365-17-9	64365179	-	-	4653														18%	-7.1	-7.4	-9.0
N-butyl-2,2,6,6-tetramethylpiperidin-4-amine, oligomeric react	500-311-6	120498-03-5	120498035	-	-	4654														18%	-7.1	-7.4	-9.0
Phenol, reaction products with 1-bromo-4-phenoxybenzene an	700-709-1	1264747-45-6	1264747456	-	-	4655														18%	-7.1	-7.4	-9.0
Benzenesulfonic acid, 4-C10-13-sec-alkyl derivs., compds. with	284-664-9	84961-74-0	84961740	-	-	4656														18%	-7.1	-7.4	-9.0
Sulfuric acid, mono-C16-18-alkyl esters, sodium salts	273-258-7	68955-20-4	68955204	-	-	4657														18%	-7.1	-7.4	-9.0
629-732-4	629-732-4	1224966-13-5	1224966135	-	-	4658														18%	-7.1	-7.4	-9.0
800-984-9	800-984-9	1428547-35-6	1428547356	-	-	4659														18%	-7.1	-7.4	-9.0
1-Pentene, chlorinated, epoxidized, distn. residues	304-798-4	94279-53-5	94279535	-	-	4660														18%	-7.1	-7.4	-9.0
Isotridecanol, ethoxylated	500-241-6	69011-36-5	69011365	-	-	4661														18%	-7.1	-7.4	-9.1
609-993-0	609-993-0	42131-25-9	42131259	-	-	4662														18%	-7.1	-7.4	-9.1
anhydro-D-glucitol trioleate	247-569-3	26266-58-0	26266580	-	-	4663														18%	-7.1	-7.4	-9.1
700-481-3	700-481-3	10257-32-6	10257326	-	-	4664														18%	-7.1	-7.4	-9.1
Rosin amine distillation fraction of disproportionated, ammoni	801-966-3	12698-87-2	12698872	-	-	4665														18%	-7.1	-7.4	-9.1
2-piperidin-2-ylethanol	216-059-2	1484-84-0	1484840	-	-	4666														18%	-7.1	-7.4	-9.1
D-Glucopyranose, oligomers, C12-14-alkyl glycosides	500-395-4	157707-88-5	157707885	-	-	4667														18%	-7.1	-7.4	-9.1
ethyl 2-(ethoxymethylene)-4,4-difluoro-3-oxobutanoate	619-794-0	176969-33-8	176969338	-	-	4668														18%	-7.1	-7.4	-9.1
1,2,3,4-tetrahydro-1-naphthylamine	218-712-7	2217-40-5	2217405	-	-	4669														18%	-7.1	-7.4	-9.1
1-ethylpyrrolidin-2-ylmethylamine	247-466-3	26116-12-1	26116121	-	-	4670														18%	-7.1	-7.4	-9.1
609-333-1	609-333-1	37143-54-7	37143547	-	-	4671														18%	-7.1	-7.4	-9.1
methylpentane	639-864-4	43133-95-5	43133955	-	-	4672														18%	-7.1	-7.4	-9.1
805-389-8	805-389-8	500011-91-6	500011916	-	-	4673														18%	-7.1	-7.4	-9.1
Methyl 3-chloro-2-fluoropropanoate	627-096-2	55900-27-1	55900271	-	-	4674														18%	-7.1	-7.4	-9.1
2,2'-(ethane-1,2-diyldiimino)bis[(2-hydroxy-5- sulfophenyl)acet	611-514-5	57368-07-7	57368077	-	-	4675														18%	-7.1	-7.4	-9.1
2-methylcyclohexanol, mixed isomers	209-512-0	583-59-5	583595	-	-	4676														18%	-7.1	-7.4	-9.1
Fatty acids, tall-oil, ethoxylated	500-150-1	61791-00-2	61791002	-	-	4677														18%	-7.1	-7.4	-9.1
1-(3-methoxyphenyl)ethanamine	700-849-3	62409-13-6	62409136	-	-	4678														18%	-7.1	-7.4	-9.1
1-(4-Methoxyphenyl)ethanamine	700-847-2	6298-96-0	6298960	-	-	4679														18%	-7.1	-7.4	-9.1
613-701-7	613-701-7	6485-45-6	6485456	-	-	4680														18%	-7.1	-7.4	-9.1
Tar bases, coal, crude	266-018-8	65996-84-1	65996841	-	-	4681														18%	-7.1	-7.4	-9.1
Sulfonic acids, alkane, sodium salts	271-774-7	68608-15-1	68608151	-	-	4682														18%	-7.1	-7.4	-9.1
N-{1-cyano-2-[5-cyano-2-(trifluoromethyl)phenoxy]-1-methylet	632-606-1	851976-50-6	851976506	-	-	4683														18%	-7.1	-7.4	-9.1
Fatty acids, tall-oil, compds. with N-[3-(dimethylamino)propyl]t	295-714-4	92128-22-8	92128228	-	-	4684														18%	-7.1	-7.4	-9.1
2-Propenoic acid, butyl ester, reaction products with butadiene	300-339-7	93925-37-2	93925372	-	-	4685														18%	-7.1	-7.4	-9.1
Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Pr)	272-723-1	68909-93-3	68909933	-	-	4686														18%	-7.1	-7.4	-9.1
Tridecanamine, N-tridecyl-, branched and linear	309-798-8	101012-97-9	101012979	-	-	4687														18%	-7.1	-7.4	-9.1
1,3,4-Thiadiazolidine-2,5-dithione, reaction products with hydr	293-927-7	91648-65-6	91648656	-	-	4688														18%	-7.1	-7.4	-9.1
Naphthenic acids, reaction products with diethylenetriamine	268-610-1	68131-13-5	68131135	-	-	4689														18%	-7.1	-7.4	-9.1
diisopropylbenzene	246-835-6	25321-09-9	25321099	-	-	4690														18%	-7.1	-7.4	-9.1
604-608-2	604-608-2	147853-32-5	147853325	-	-	4691														18%	-7.1	-7.4	-9.1
3,7-dimethylnona-1,6-dien-3-ol	233-732-6	10339-55-6	10339556	-	-	4692														18%	-7.1	-7.4	-9.1
696-616-8	696-616-8	1268344-02-0	1268344020	-	-	4693														18%	-7.1	-7.4	-9.1
606-330-7	606-330-7	195008-76-5	195008765	-	-	4694														18%	-7.1	-7.4	-9.1
sucrose di(acetate) hexaisobutyrate	204-771-6	126-13-6	126136	-	-	4695														18%	-7.1	-7.4	-9.1
Alcohols, C9-11, branched and linear, ethoxylated, sulfates, am	500-464-9	160901-27-9	160901279	-	-	4696														18%	-7.1	-7.4	-9.1
629-765-4	629-765-4	1226892-44-9	1226892449	-	-	4697														18%	-7.1	-7.4	-9.1
Fatty acids, C8-10, C12-18-alkyl esters	306-082-7	95912-86-0	95912860	-	-	4698														18%	-7.1	-7.4	-9.1
Cellulase	232-734-4	9012-54-8	9012548	-	-	4699														18%	-7.1	-7.4	-9.1
2-propylheptyl acrylate	604-669-5	149021-58-9	149021589	-	-	4700														18%	-7.1	-7.5	-9.1
1,2,3,6-Tetrahydrophthalic anhydride, oligomeric reaction proc	500-091-1	36621-20-2	36621202	-	-	4701														18%	-7.1	-7.5	-9.1
2,4,6-tri-sec-butylphenol	227-572-6	5892-47-7	5892477	-	-	4702														18%	-7.1	-7.5	-9.1
Soaps, stocks, acidulated	271-768-4	68607-87-4	68607874	-	-	4703														18%	-7.1	-7.5	-9.1
Quaternary ammonium compounds, bis(hydrogenated tallow a	272-745-1	68910-55-4	68910554	-	-	4704														18%	-7.1	-7.5	-9.1
Rosin, fumarated, reaction products with formaldehyde	305-795-0	95009-65-7	95009657	-	-	4705														18%	-7.1	-7.5	-9.1
Humic acids, sodium salts	268-608-0	68131-04-4	68131044	-	-	4706														18%	-7.1	-7.5	-9.1

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Phosphoric acid, 2-ethylhexyl ester	235-741-0	12645-31-7	12645317	-	-	4707														18%	-7.2	-7.5	-9.1
Pentaerythritol, ethoxylated	500-071-2	30599-15-6	30599156	-	-	4708														18%	-7.2	-7.5	-9.1
Benzenamine, N-phenyl-, reaction products with styrene and 2,	272-940-1	68921-45-9	68921459	-	-	4709														18%	-7.2	-7.5	-9.1
Mentha arvensis, ext.	290-058-5	90063-97-1	90063971	-	-	4710														18%	-7.2	-7.5	-9.1
1-Octadecanol, phosphate, potassium salt	273-489-3	68987-29-1	68987291	-	-	4711														18%	-7.2	-7.5	-9.1
Fatty acids, C8-10, tetraesters with pentaerythritol	287-827-2	85586-24-9	85586249	-	-	4712														18%	-7.2	-7.5	-9.1
Lemon, ext.	284-515-8	84929-31-7	84929317	-	-	4713														18%	-7.2	-7.5	-9.1
Fatty acids, C16-18, Bu esters	287-039-9	85408-76-0	85408760	-	-	4714														18%	-7.2	-7.5	-9.1
2,4-Pentanedione, peroxide	253-384-9	37187-22-7	37187227	-	-	4715														18%	-7.2	-7.5	-9.1
Oils, fish, sulfated, sodium salts	262-992-3	61788-64-5	61788645	-	-	4716														18%	-7.2	-7.5	-9.1
Fatty acids, C16-18 and C18 unsatd., triesters with trimethylolp	268-092-7	68002-78-8	68002788	-	-	4717														18%	-7.2	-7.5	-9.1
Soybean oil, deodorizer distillate	272-211-8	68783-88-0	68783880	-	-	4718														18%	-7.2	-7.5	-9.1
α,α,α',α'-tetramethylxylene-α,α-diol	248-256-4	27138-01-8	27138018	-	-	4719														18%	-7.2	-7.5	-9.1
614-637-2	614-637-2	68603-75-8	68603758	-	-	4720														18%	-7.2	-7.5	-9.1
Fatty acids, C6-18, triesters with trimethylolpropane	293-035-8	91050-88-3	91050883	-	-	4721														18%	-7.2	-7.5	-9.1
Castor oil, dehydrated	264-705-7	64147-40-6	64147406	-	-	4722														18%	-7.2	-7.5	-9.1
800-526-8	800-526-8	1273322-45-4	1273322454	-	-	4723														18%	-7.2	-7.5	-9.1
disodium oxybis[methylbenzenesulphonate]	277-242-0	73037-34-0	73037340	-	-	4724														18%	-7.2	-7.5	-9.2
Amines, C11-14-branched alkyl, monohexyl and dihexyl phosph	279-632-6	80939-62-4	80939624	-	-	4725														18%	-7.2	-7.5	-9.2
605-143-8	605-143-8	158318-67-3	158318673	-	-	4726														18%	-7.2	-7.5	-9.2
601-566-7	601-566-7	118800-30-9	118800309	-	-	4727														18%	-7.2	-7.5	-9.2
Aromatic hydrocarbons, C6-10, C8-rich	292-697-5	90989-41-6	90989416	-	-	4728														18%	-7.2	-7.5	-9.2
Fatty acids, C8-18 and C18-unsatd., esters with pentaerythritol	285-202-9	85049-33-8	85049338	-	-	4729														18%	-7.2	-7.5	-9.2
Alcohols, C9-11, branched and linear, ethoxylated	500-446-0	160901-09-7	160901097	-	-	4730														18%	-7.2	-7.5	-9.2
4,4'-Isopropylidenediphenol, oligomeric reaction products with	500-180-5	67989-52-0	67989520	-	-	4731														18%	-7.2	-7.5	-9.2
800-838-4	800-838-4	1384855-91-7	1384855917	-	-	4732														18%	-7.2	-7.5	-9.2
Soybean oil, epoxidized, acrylate	294-415-6	91722-14-4	91722144	-	-	4733														18%	-7.2	-7.5	-9.2
Ethylenediamine, ethoxylated and propoxylated	500-047-1	26316-40-5	26316405	-	-	4734														18%	-7.2	-7.5	-9.2
decene	246-870-7	25339-53-1	25339531	-	-	4735														18%	-7.2	-7.5	-9.2
608-670-1	608-670-1	31831-53-5	31831535	-	-	4736														18%	-7.2	-7.5	-9.2
Alcohols, C8-14, γ-ω-perfluoro	269-927-8	68391-08-2	68391082	-	-	4737														18%	-7.2	-7.5	-9.2
triisodecyl phosphite	246-998-3	25448-25-3	25448253	-	-	4738														18%	-7.2	-7.5	-9.2
Fatty acids, dehydrated castor-oil	263-061-4	61789-45-5	61789455	-	-	4739														18%	-7.2	-7.5	-9.2
9-Octadecenoic acid (Z)-, monoester with 1,2,3-propanetriol es	264-092-6	63310-16-7	63310167	-	-	4740														18%	-7.2	-7.5	-9.2
609-946-4	609-946-4	41637-38-1	41637381	-	-	4741														18%	-7.2	-7.5	-9.2
Petrolatum (petroleum), oxidized, calcium salt	270-348-8	68425-34-3	68425343	-	-	4742														18%	-7.2	-7.5	-9.2
Hydrocarbons, terpene processing by-products	273-309-3	68956-56-9	68956569	-	-	4743														18%	-7.2	-7.5	-9.2
614-279-7	614-279-7	68122-64-5	68122645	-	-	4744														18%	-7.2	-7.5	-9.2
619-057-3	619-057-3	94667-33-1	94667331	-	-	4745														18%	-7.2	-7.5	-9.2
Fatty acids, C5-9, tetraesters with pentaerythritol	267-022-2	67762-53-2	67762532	-	-	4746														18%	-7.2	-7.5	-9.2
1,2-Benzenedicarboxylic acid, di-C8-10-alkyl esters	275-809-7	71662-46-9	71662469	-	-	4747														18%	-7.3	-7.6	-9.2
616-261-4	616-261-4	75782-87-5	75782875	-	-	4748														18%	-7.3	-7.6	-9.2
Extract residues (coal), tar oil alk.	266-021-4	65996-87-4	65996874	-	-	4749														18%	-7.3	-7.6	-9.2
2,2,4,4-tetramethylcyclobutane-1,3-diol, mixed isomers	221-140-0	3010-96-6	3010966	-	-	4750														18%	-7.3	-7.6	-9.2
Phenol, dodecyl-, branched, sulfurized	306-115-5	96152-43-1	96152431	-	-	4751														18%	-7.3	-7.6	-9.2
1,2,3-propanetriyl trioleate	204-534-7	122-32-7	122327	-	-	4752														18%	-7.3	-7.6	-9.2
Resin acids and Rosin acids, reaction products with formaldehy	295-855-1	92129-53-8	92129538	-	-	4753														18%	-7.3	-7.6	-9.2
Castor oil, ethoxylated	500-151-7	61791-12-6	61791126	-	-	4754														18%	-7.3	-7.6	-9.2
Soybean oil, epoxidized, ether with ethylene glycol	287-836-1	85586-34-1	85586341	-	-	4755														18%	-7.3	-7.6	-9.2
Reaction products of benzene-1,4-diamine and methyl 2,3,4,5-t	600-736-8	106276-80-6	106276806	-	-	4756														18%	-7.3	-7.6	-9.2
Acacia mearnsi, ext., reaction products with ammonium chloric	285-077-0	85029-52-3	85029523	-	-	4757														18%	-7.3	-7.6	-9.2
Fatty acids, C14-18 and C16-18-unsatd., mixed esters with neop	286-078-9	85186-92-1	85186921	-	-	4758														18%	-7.3	-7.6	-9.2
Phosphoric acid, C16-18-alkyl esters, potassium salts	291-907-2	90506-45-9	90506459	-	-	4759														18%	-7.3	-7.6	-9.2
2-[[2,2-bis[[(1-oxoallyl)oxy]methyl]butoxy]methyl]-2-ethyl-1,3-p	302-434-9	94108-97-1	94108971	-	-	4760														18%	-7.3	-7.6	-9.2
629-742-9	629-742-9	1226892-49-4	1226892494	-	-	4761														18%	-7.3	-7.6	-9.2
Fatty acids, C5-9, hexaesters with dipentaerythritol	267-021-7	67762-52-1	67762521	-	-	4762														18%	-7.3	-7.6	-9.2
Fatty acids, C14-18 and C16-18-unsatd., maleated	288-306-2	85711-46-2	85711462	-	-	4763														18%	-7.3	-7.6	-9.2
614-295-4	614-295-4	68131-40-8	68131408	-	-	4764														18%	-7.3	-7.6	-9.2
Polyphosphoric acids, esters with triethanolamine, sodium salt	268-625-3	68131-72-6	68131726	-	-	4765														18%	-7.3	-7.6	-9.3
Castor oil, oxidized	269-128-4	68187-84-8	68187848	-	-	4766														18%	-7.3	-7.6	-9.3
604-394-0	604-394-0	144086-02-2	144086022	-	-	4767														18%	-7.3	-7.6	-9.3
4,4'-Isopropylidenediphenol, oligomeric reaction products with	500-181-0	68002-42-6	68002426	-	-	4768														18%	-7.3	-7.6	-9.3
titanium tetra(octanolate), branched and linear	281-199-3	83897-91-0	83897910	-	-	4769														18%	-7.3	-7.6	-9.3
607-759-2	607-759-2	25618-55-7	25618557	-	-	4770														18%	-7.3	-7.6	-9.3
1,2-Benzenedicarboxylic acid, di-C6-10-alkyl esters	271-094-0	68515-51-5	68515515	-	-	4771														18%	-7.3	-7.6	-9.3
2-Propanol, 1,1'-[[3-[(3-aminopropyl)amino]propyl]imino]bis-,	307-276-4	97592-79-5	97592795	-	-	4772														18%	-7.3	-7.6	-9.3
Phosphoric acid, dodecyl ester, potassium salt	254-414-3	39322-78-6	39322786	-	-	4773														18%	-7.3	-7.6	-9.3
Fatty acids, C16-18, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester	292-947-3	91031-45-7	91031457	-	-	4774														18%	-7.3	-7.6	-9.3
Amines, N-C12-14-alkyltrimethylenedi-	292-562-0	90640-43-0	90640430	-	-	4775														18%	-7.3	-7.6	-9.3
Protein hydrolyzates, vegetable	309-353-8	100209-45-8	100209458	-	-	4776														18%	-7.3	-7.6	-9.3
2-Propenoic acid, γ-ω-perfluoro-C8-14-alkyl esters	288-003-5	85631-54-5	85631545	-	-	4777														18%	-7.3	-7.6	-9.3
Amines, di-C12-18-alkyl	268-899-4	68153-95-7	68153957	-	-	4778														18%	-7.3	-7.6	-9.3
3,7,11-trimethyldodeca-1,6,10-trien-3-ol,mixed isomers	230-597-5	7212-44-4	7212444	-	-	4779														18%	-7.3	-7.6	-9.3
tetradecyl oleate	244-949-0	22393-85-7	22393857	-	-	4780														18%	-7.3	-7.6	-9.3
1,3-dihydro-4(or 5)-methyl-2H-benzimidazole-2-thione	258-904-8	53988-10-6	53988106	-	-	4781														18%	-7.3	-7.6	-9.3

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
615-086-0	615-086-0	70225-05-7	70225057	-	-	4782														18%	-7.3	-7.6	-9.3
Acetic acid, oxo-, sodium salt, reaction products with cresol and	283-041-9	84539-53-7	84539537	-	-	4783														18%	-7.3	-7.6	-9.3
Fatty acids, C16-18 and C18-unsatd., compds. with triethanolar	270-279-3	68424-19-1	68424191	-	-	4784														18%	-7.3	-7.6	-9.3
Docosanoic acid, ester with 1,2,3-propanetriol	278-717-5	77538-19-3	77538193	-	-	4785														18%	-7.3	-7.6	-9.3
Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu)	270-478-5	68442-22-8	68442228	-	-	4786														18%	-7.3	-7.6	-9.3
diisopropylbenzene hydroperoxide	247-988-1	26762-93-6	26762936	-	-	4787														18%	-7.3	-7.6	-9.3
Resin acids and Rosin acids, fumarated, esters with glycerol	307-051-0	97489-11-7	97489117	-	-	4788														18%	-7.3	-7.6	-9.3
sodium N-(2-carboxyethyl)-N-(2-ethylhexyl)-β-alaninate	305-318-6	94441-92-6	94441926	-	-	4789														18%	-7.3	-7.6	-9.3
Amides, C16-18 and C18-unsatd., N,N-bis(hydroxyethyl)	271-653-9	68603-38-3	68603383	-	-	4790														18%	-7.3	-7.6	-9.3
4,4'-Methylenedianiline, oligomeric reaction products with 1-cl	500-062-3	28390-91-2	28390912	-	-	4791														18%	-7.3	-7.6	-9.3
Fatty acids, C16-18, tetraesters with pentaerythritol	293-029-5	91050-82-7	91050827	-	-	4792														18%	-7.3	-7.7	-9.3
694-886-1	694-886-1	1365095-43-7	1365095437	-	-	4793														18%	-7.3	-7.7	-9.3
614-523-2	614-523-2	68475-37-6	68475376	-	-	4794														18%	-7.3	-7.7	-9.3
tert-butyl peroxyneodecanoate	247-955-1	26748-41-4	26748414	-	-	4795														18%	-7.4	-7.7	-9.3
Tar acids, distn. residues	306-251-5	96690-55-0	96690550	-	-	4796														18%	-7.4	-7.7	-9.3
Amines, C16-18-alkyldimethyl	269-915-2	68390-97-6	68390976	-	-	4797														18%	-7.4	-7.7	-9.3
Fatty acids, C12-16, esters with neopentyl glycol	286-081-5	85186-95-4	85186954	-	-	4798														18%	-7.4	-7.7	-9.3
Naphthalenesulfonic acids, branched and linear Bu derivs., sod	293-346-9	91078-64-7	91078647	-	-	4799														18%	-7.4	-7.7	-9.3
Alcohols, C6-24 and C6-24-unsatd., distn. residues	310-079-6	102242-48-8	102242488	-	-	4800														18%	-7.4	-7.7	-9.3
docosyl docosanoate	241-646-5	17671-27-1	17671271	-	-	4801														18%	-7.4	-7.7	-9.3
Glycerides, C16-18 mono-, di- and tri-, hydrogenated, citrates,	294-600-1	91744-38-6	91744386	-	-	4802														18%	-7.4	-7.7	-9.3
606-078-8	606-078-8	186321-96-0	186321960	-	-	4803														18%	-7.4	-7.7	-9.3
800-660-7	800-660-7	1258274-08-6	1258274086	-	-	4804														18%	-7.4	-7.7	-9.3
Fatty acids, tall-oil, C12-15-alkyl esters, sulfated, sodium salts	270-307-4	68424-50-0	68424500	-	-	4805														18%	-7.4	-7.7	-9.3
Fatty acids, tallow, zinc salts	270-451-8	68440-34-6	68440346	-	-	4806														18%	-7.4	-7.7	-9.3
d-Glucose, ether with glycerol	309-496-6	100402-60-6	100402606	-	-	4807														18%	-7.4	-7.7	-9.3
610-877-7	610-877-7	52624-57-4	52624574	-	-	4808														18%	-7.4	-7.7	-9.3
2,2-bis[[(1-oxoisooctadecyl)oxy]methyl]-1,3-propanediyl bis(isc	263-423-1	62125-22-8	62125228	-	-	4809														18%	-7.4	-7.7	-9.3
Alcohols, C9-11, branched and linear, ethoxylated, sulfates, soc	500-465-4	160901-28-0	160901280	-	-	4810														18%	-7.4	-7.7	-9.3
(1α,2β,4β,6α)-2,2,7-trimethyl-3-oxatricyclo[4.1.1.02,4]octane	250-938-1	32162-27-9	32162279	-	-	4811														18%	-7.4	-7.7	-9.3
629-723-5	629-723-5	1190409-68-7	1190409687	-	-	4812														18%	-7.4	-7.7	-9.3
806-510-7	806-510-7	1393571-43-1	1393571431	-	-	4813														18%	-7.4	-7.7	-9.3
629-716-7	629-716-7	1211950-04-7	1211950047	-	-	4814														18%	-7.4	-7.7	-9.3
diisodecyl sebacate	249-047-0	28473-19-0	28473190	-	-	4815														18%	-7.4	-7.7	-9.4
800-172-4	800-172-4	398141-87-2	398141872	-	-	4816														18%	-7.4	-7.7	-9.4
Butanedioic acid, sulfo-, 1-C12-18-alkyl esters, disodium salts	290-836-4	90268-36-3	90268363	-	-	4817														18%	-7.4	-7.7	-9.4
Distillates (coal tar), pitch	309-855-7	101316-49-8	101316498	-	-	4818														18%	-7.4	-7.7	-9.4
606-155-6	606-155-6	188831-96-1	188831961	-	-	4819														18%	-7.4	-7.7	-9.4
Phosphoric acid, octadecyl ester	254-466-7	39471-52-8	39471528	-	-	4820														18%	-7.4	-7.7	-9.4
Amines, tallow alkyl, dodecylbenzenesulfonates	268-766-0	68139-94-6	68139946	-	-	4821														18%	-7.4	-7.7	-9.4
Fatty acids, tall-oil, reaction products with formaldehyde and (2	272-789-1	68911-83-1	68911831	-	-	4822														18%	-7.4	-7.7	-9.4
Peptones, casein	293-428-4	91079-40-2	91079402	-	-	4823														18%	-7.4	-7.7	-9.4
zinc bis[bis(tetrapropylenephenyl)] bis(hydrogen dithiophosph	234-277-6	11059-65-7	11059657	-	-	4824														18%	-7.4	-7.7	-9.4
cyclohexane-1,4-dicarboxylic acid	214-068-6	1076-97-7	1076977	-	-	4825														18%	-7.4	-7.7	-9.4
4,4'-Isopropylidenediphenol, oligomeric reaction products with	500-655-7	161308-15-2	161308152	-	-	4826														18%	-7.4	-7.7	-9.4
604-766-2	604-766-2	151006-58-5	151006585	-	-	4827														18%	-7.4	-7.7	-9.4
β-Alanine, N-(2-carboxyethyl)-, N-coco alkyl derivs., disodium s	290-476-8	90170-43-7	90170437	-	-	4828														18%	-7.4	-7.7	-9.4
613-583-7	613-583-7	64366-79-6	64366796	-	-	4829														18%	-7.4	-7.7	-9.4
Fatty acids, C16-18 and C18-unsatd., Et esters	285-206-0	85049-36-1	85049361	-	-	4830														18%	-7.4	-7.7	-9.4
Resin acids and Rosin acids, esters with diethylene glycol	268-884-2	68153-38-8	68153388	-	-	4831														18%	-7.4	-7.7	-9.4
2,2-dimethyl-1,3-propanediyl dioleate	255-713-1	42222-50-4	42222504	-	-	4832														18%	-7.4	-7.7	-9.4
Tar acids, 3,5-xylenol fraction	284-896-0	84989-07-1	84989071	-	-	4833														18%	-7.4	-7.8	-9.4
628-862-9	628-862-9	1219458-11-3	1219458113	-	-	4834														18%	-7.4	-7.8	-9.4
Decanol, branched and linear	291-169-1	90342-32-8	90342328	-	-	4835														18%	-7.4	-7.8	-9.4
Nitric acid, reaction products with cyclododecanol and cyclodo	276-431-5	72162-23-3	72162233	-	-	4836														18%	-7.4	-7.8	-9.4
3,4,5,5-tetramethylhex-2-ene	254-281-1	39083-38-0	39083380	-	-	4837														18%	-7.5	-7.8	-9.4
614-270-8	614-270-8	68082-79-1	68082791	-	-	4838														18%	-7.5	-7.8	-9.4
1,4-butanediylbis[oxy(2-hydroxy-3,1-propanediyl)] diacrylate	257-900-3	52408-42-1	52408421	-	-	4839														18%	-7.5	-7.8	-9.4
Glycerides, C12-18 di- and tri-	294-590-9	91744-28-4	91744284	-	-	4840														18%	-7.5	-7.8	-9.4
Resin acids and Rosin acids, maleated, esters with pentaerythri	305-516-2	94581-17-6	94581176	-	-	4841														18%	-7.5	-7.8	-9.4
605-293-4	605-293-4	162568-25-4	162568254	-	-	4842														18%	-7.5	-7.8	-9.4
1,2-dichloro-1,1,2-trifluoro-2-(trifluoromethoxy)ethane	219-094-1	2356-53-8	2356538	-	-	4843														18%	-7.5	-7.8	-9.4
1,2,4-Benzenetricarboxylic acid, tri-C9-11-alkyl esters	304-780-6	94279-36-4	94279364	-	-	4844														18%	-7.5	-7.8	-9.4
Fatty acids, C16-18, lithium salts	272-195-2	68783-37-9	68783379	-	-	4845														18%	-7.5	-7.8	-9.4
Fatty acids, C14-18 and C16-18-unsatd., esters with neopentyl	285-533-9	85116-81-0	85116810	-	-	4846														18%	-7.5	-7.8	-9.4
β-Alanine, N-C8-18-alkyl derivs., monopotassium salts	290-475-2	90170-42-6	90170426	-	-	4847														18%	-7.5	-7.8	-9.4
4,4'-Isopropylidenediphenol, polymer with 1-chloro-2,3-epoxyp	500-240-0	68958-77-0	68958770	-	-	4848														18%	-7.5	-7.8	-9.4
Fatty acids, vegetable-oil, sulfated, sodium salts	262-996-5	61788-67-8	61788678	-	-	4849														18%	-7.5	-7.8	-9.4
zinc O,O,O',O'-tetrabutyl bis(phosphorodithioate)	230-257-6	6990-43-8	6990438	-	-	4850														18%	-7.5	-7.8	-9.5
Pentaerythritol, ethoxylated and propoxylated	500-069-1	30374-35-7	30374357	-	-	4851														18%	-7.5	-7.8	-9.5
9-Octadecenoic acid (Z)-, reaction products with 2-[(2-aminoet	272-379-2	68815-51-0	68815510	-	-	4852														18%	-7.5	-7.8	-9.5
Quaternary ammonium compounds, tri-C8-10-alkylmethyl, chlo	264-120-7	63393-96-4	63393964	-	-	4853														18%	-7.5	-7.8	-9.5
Benzene, ethylenated, by-products from	271-802-8	68608-82-2	68608822	-	-	4854														18%	-7.5	-7.8	-9.5
Amines, C16-22-alkyl	268-215-4	68037-92-3	68037923	-	-	4855														18%	-7.5	-7.8	-9.5
Fatty acids, C18-unsatd., reaction products with acrylic acid and	287-820-4	85586-18-1	85586181	-	-	4856														18%	-7.5	-7.8	-9.5

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
bis(tridecyl) adipate	241-029-0	16958-92-2	16958922	-	-	4857														18%	-7.5	-7.8	-9.5
sodium N-methyl-N-(1-oxo-9-octadecenyl)aminoacetate	222-829-9	3624-77-9	3624779	-	-	4858														18%	-7.5	-7.8	-9.5
Phenol, dodecyl-, sulfurized, carbonates, calcium salts	272-233-8	68784-25-8	68784258	-	-	4859														18%	-7.5	-7.8	-9.5
Fatty acids, C14-18 and C16-18-unsatd., esters with propylene	284-864-6	84988-75-0	84988750	-	-	4860														18%	-7.5	-7.8	-9.5
629-767-5	629-767-5	1228186-18-2	1228186182	-	-	4861														18%	-7.5	-7.8	-9.5
800-309-8	800-309-8	231297-75-9	231297759	-	-	4862														18%	-7.5	-7.8	-9.5
Amines, (C16-18 and C18-unsatd. alkyl)dimethyl	268-220-1	68037-96-7	68037967	-	-	4863														18%	-7.5	-7.8	-9.5
Paraffin waxes and Hydrocarbon waxes, oxidized, lithium salts	272-032-5	68649-48-9	68649489	-	-	4864														18%	-7.5	-7.8	-9.5
Fatty acids, C18-unsatd., dimers, methyl esters	500-225-9	68604-84-2	68604842	-	-	4865														18%	-7.5	-7.8	-9.5
Fatty acids, C16-18, reaction products with diethanolamine	293-014-3	91032-08-5	91032085	-	-	4866														18%	-7.5	-7.8	-9.5
Sorbitan monolaurate, ethoxylated	500-018-3	9005-64-5	9005645	-	-	4867														18%	-7.5	-7.8	-9.5
610-945-6	610-945-6	53037-34-6	53037346	-	-	4868														18%	-7.5	-7.8	-9.5
Fatty acids, lanolin, esters with pentaerythritol	270-434-5	68440-09-5	68440095	-	-	4869														18%	-7.5	-7.8	-9.5
N,N'-ethane-1,2-diylbisoleamide	203-756-1	110-31-6	110316	-	-	4870														18%	-7.5	-7.8	-9.5
615-240-7	615-240-7	710292-85-6	710292856	-	-	4871														18%	-7.5	-7.8	-9.5
Amines, C12-14-tert-alkyl	273-279-1	68955-53-3	68955533	-	-	4872														18%	-7.5	-7.8	-9.5
sodium 4(or 5)-methyl-1H-benzotriazolide	265-004-9	64665-57-2	64665572	-	-	4873														18%	-7.5	-7.9	-9.5
isooctyl mercaptoacetate	246-613-9	25103-09-7	25103097	-	-	4874														18%	-7.5	-7.9	-9.5
orthoboric acid, compound with 2,2'-iminodiethanol	267-886-0	67952-33-4	67952334	-	-	4875														18%	-7.5	-7.9	-9.5
(octadecanoato-O)oxoaluminium	236-521-7	13419-15-3	13419153	-	-	4876														18%	-7.5	-7.9	-9.5
dihydro-3-(octenyl)furan-2,5-dione	247-899-8	26680-54-6	26680546	-	-	4877														18%	-7.5	-7.9	-9.5
Amines, C12-16-alkyldimethyl	270-414-6	68439-70-3	68439703	-	-	4878														18%	-7.5	-7.9	-9.5
Benzenesulfonic acid, mono-C11-13-branched alkyl derivs., sod	271-808-0	68608-89-9	68608899	-	-	4879														18%	-7.6	-7.9	-9.5
Fatty acids, C16-18, 2-octyldodecyl esters	306-232-1	96690-38-9	96690389	-	-	4880														18%	-7.6	-7.9	-9.5
Cyclohexane, oxidized, distillates	308-380-2	97952-85-7	97952857	-	-	4881														18%	-7.6	-7.9	-9.5
Resin acids and Rosin acids, fumarated, compds. with triethanc	293-625-5	91081-22-0	91081220	-	-	4882														18%	-7.6	-7.9	-9.5
N-octadecylstearamide	236-276-6	13276-08-9	13276089	-	-	4883														18%	-7.6	-7.9	-9.5
Pyridine, alkyl derivs.	269-929-9	68391-11-7	68391117	-	-	4884														18%	-7.6	-7.9	-9.5
Cashew, nutshell liq., oligomeric reaction products with 1-chlor	500-210-7	68413-24-1	68413241	-	-	4885														18%	-7.6	-7.9	-9.5
Rape oil, sulfated, ammonium salt	281-976-7	84082-28-0	84082280	-	-	4886														18%	-7.6	-7.9	-9.5
Glycerides, C16-18 mono-, di- and tri-	293-215-6	91052-54-9	91052549	-	-	4887														18%	-7.6	-7.9	-9.5
610-848-9	610-848-9	52479-58-0	52479580	-	-	4888														18%	-7.6	-7.9	-9.5
800-426-4	800-426-4	1373883-45-4	1373883454	-	-	4889														18%	-7.6	-7.9	-9.5
isooctadecan-1-ol	248-470-8	27458-93-1	27458931	-	-	4890														18%	-7.6	-7.9	-9.5
Fatty acids, C16-18, iso-Pr esters	292-962-5	91031-58-2	91031582	-	-	4891														18%	-7.6	-7.9	-9.5
isodecyl oleate	261-673-6	59231-34-4	59231344	-	-	4892														18%	-7.6	-7.9	-9.5
603-188-8	603-188-8	127184-53-6	127184536	-	-	4893														18%	-7.6	-7.9	-9.5
Fatty acids, C16-18 and C18-unsatd., hexaesters with dipentaer	271-689-5	68604-38-6	68604386	-	-	4894														18%	-7.6	-7.9	-9.5
Glycerides, mixed coco, decanoyl and octanoyl	271-729-1	68606-18-8	68606188	-	-	4895														18%	-7.6	-7.9	-9.5
676-712-6	676-712-6	68890-85-7	68890857	-	-	4896														18%	-7.6	-7.9	-9.5
607-997-7	607-997-7	26776-30-7	26776307	-	-	4897														18%	-7.6	-7.9	-9.6
4,4'-Isopropylidenediphenol, oligomeric reaction products with	500-302-7	113930-69-1	113930691	-	-	4898														18%	-7.6	-7.9	-9.6
1,2-Ethanediamine, N-(2-aminoethyl)-, reaction products with	291-221-3	90366-78-2	90366782	-	-	4899														18%	-7.6	-7.9	-9.6
Alkenes, C15-18 α-, sulfurized	267-023-8	67762-55-4	67762554	-	-	4900														18%	-7.6	-7.9	-9.6
607-907-6	607-907-6	26301-10-0	26301100	-	-	4901														18%	-7.6	-7.9	-9.6
isopropylnaphthalene	249-535-3	29253-36-9	29253369	-	-	4902														18%	-7.6	-7.9	-9.6
Peppermint, ext.	282-015-4	84082-70-2	84082702	-	-	4903														18%	-7.6	-7.9	-9.6
Glycerides, C10-20 and C10-20-unsatd., oxidized	295-734-3	92128-40-0	92128400	-	-	4904														18%	-7.6	-7.9	-9.6
2-Butenedioic acid (E)-, di-C12-18-alkyl esters	272-943-8	68921-51-7	68921517	-	-	4905														18%	-7.6	-7.9	-9.6
Phosphoric acid, mono- and bis(branched and linear pentyl) est	282-784-6	84418-71-3	84418713	-	-	4906														18%	-7.6	-7.9	-9.6
Benzene-1,2,4-tricarboxylic acid 1,2-anhydride, oligomeric reac	500-199-9	68183-39-1	68183391	-	-	4907														18%	-7.6	-7.9	-9.6
Fatty acids, tall-oil, reaction products with ethanolamine	270-445-5	68440-25-5	68440255	-	-	4908														18%	-7.6	-7.9	-9.6
Distillates (coal tar), naphthalene oils, methylnaphthalene fract	309-985-4	101896-27-9	101896279	-	-	4909														18%	-7.6	-7.9	-9.6
Fatty acids, C18-unsatd., dimers, hydrogenated, dimethyl ester	500-449-7	160901-12-2	160901122	-	-	4910														18%	-7.6	-7.9	-9.6
605-315-2	605-315-2	163149-28-8	163149288	-	-	4911														18%	-7.6	-7.9	-9.6
614-560-4	614-560-4	68517-10-2	68517102	-	-	4912														18%	-7.6	-7.9	-9.6
Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, [[	279-767-0	81457-65-0	81457650	-	-	4913														18%	-7.6	-7.9	-9.6
641-088-6	641-088-6	1229648-98-9	1229648989	-	-	4914														18%	-7.6	-7.9	-9.6
1,1-dimethylheptanethiol	246-896-9	25360-10-5	25360105	-	-	4915														18%	-7.6	-7.9	-9.6
2-ethylhexanoic acid, monoester with propane-1,2-diol	285-503-5	85114-00-7	85114007	-	-	4916														18%	-7.6	-7.9	-9.6
Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, [[	270-096-9	68411-04-1	68411041	-	-	4917														18%	-7.6	-7.9	-9.6
Fatty acids, C16-18, barium salts	292-883-6	91002-07-2	91002072	-	-	4918														18%	-7.6	-7.9	-9.6
(1-methylethyl)-1,1'-biphenyl	247-156-8	25640-78-2	25640782	-	-	4919														18%	-7.6	-7.9	-9.6
Alcohols, C12-18, ethoxylated	500-201-8	68213-23-0	68213230	-	-	4920														18%	-7.6	-7.9	-9.6
Reaction products of tall oil fatty acids with diethylenetriamine	800-430-6	1419212-76-2	1419212762	-	-	4921														18%	-7.6	-7.9	-9.6
1H-Imidazole-1-ethanol, 4,5-dihydro-, 2-nortall-oil alkyl derivs.	263-171-2	61791-39-7	61791397	-	-	4922														18%	-7.6	-7.9	-9.6
613-333-7	613-333-7	63705-03-3	63705033	-	-	4923														18%	-7.6	-7.9	-9.6
Glycerides, C8-18	287-487-5	85536-06-7	85536067	-	-	4924														18%	-7.6	-7.9	-9.6
Quaternary ammonium compounds, (C16-18 and C18-unsatd.	268-074-9	68002-61-9	68002619	-	-	4925														18%	-7.6	-8.0	-9.6
Sorbitan, (Z)-9-octadecenoate (2:3)	232-360-1	8007-43-0	8007430	-	-	4926														18%	-7.6	-8.0	-9.6
604-612-4	604-612-4	147900-93-4	147900934	-	-	4927														18%	-7.6	-8.0	-9.6
l-Glutamic acid, N-coco acyl derivs., disodium salts	269-085-1	68187-30-4	68187304	-	-	4928														18%	-7.6	-8.0	-9.6
Glycerides, C16-18 mono-, di- and tri-, hydrogenated, citrates,	294-601-7	91744-39-7	91744397	-	-	4929														18%	-7.6	-8.0	-9.6
4,4'-Isopropylidenediphenol, oligomeric reaction products with	500-090-6	36425-16-8	36425168	-	-	4930														18%	-7.6	-8.0	-9.6
Glycerides, palm-oil mono- and di-, hydrogenated	267-057-3	67784-87-6	67784876	-	-	4931														18%	-7.6	-8.0	-9.6

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Fatty acids, C16-18, iso-Bu esters	288-668-1	85865-69-6	85865696	-	-	4932														18%	-7.7	-8.0	-9.6
Fatty acids, tall-oil, reaction products with pentaethylenehexan	288-927-9	85940-40-5	85940405	-	-	4933														18%	-7.7	-8.0	-9.6
1,3-dihydro-4(or 5)-methyl-2H-benzimidazole-2-thione, zinc sal	262-872-0	61617-00-3	61617003	-	-	4934														18%	-7.7	-8.0	-9.6
Fatty acids, C14-18 and C18-unsatd., branched and linear, Me e	286-065-8	85186-80-7	85186807	-	-	4935														18%	-7.7	-8.0	-9.6
Pyridinium, 1-(phenylmethyl)-, ethyl methyl derivs., chlorides	272-695-0	68909-18-2	68909182	-	-	4936														18%	-7.7	-8.0	-9.6
Fatty acids, C16-18 and C18-unsatd., esters with pentaerythritc	288-305-7	85711-45-1	85711451	-	-	4937														18%	-7.7	-8.0	-9.6
628-863-4	628-863-4	1219458-14-6	1219458146	-	-	4938														18%	-7.7	-8.0	-9.6
1,3-Cyclohexanedimethanamine	219-941-5	2579-20-6	2579206	-	-	4939														18%	-7.7	-8.0	-9.6
Reaction products of coconut oil with polyethyleneglycol and 2-	640-964-5	218451-68-4	218451684	-	-	4940														18%	-7.7	-8.0	-9.6
Nitriles, C16-22	268-861-7	68153-02-6	68153026	-	-	4941														18%	-7.7	-8.0	-9.6
Amides, tall-oil fatty, N,N-di-Me	269-665-4	68308-74-7	68308747	-	-	4942														18%	-7.7	-8.0	-9.6
Ethanesulfonic acid, 2-(methylamino)-, N-coco acyl derivs., sodi	263-174-9	61791-42-2	61791422	-	-	4943														18%	-7.7	-8.0	-9.6
Alcohols, C12-18, ethoxylated, sulfates, sodium salts	500-189-4	68081-91-4	68081914	-	-	4944														18%	-7.7	-8.0	-9.6
629-735-0	629-735-0	1226892-50-7	1226892507	-	-	4945														18%	-7.7	-8.0	-9.6
Fatty acids, C18-unsatd., dimers, oligomeric reaction products v	500-382-3	157707-73-8	157707738	-	-	4946														18%	-7.7	-8.0	-9.6
612-396-8	612-396-8	61791-19-3	61791193	-	-	4947														18%	-7.7	-8.0	-9.6
Phosphonic acid, mixed C12-20-alkyl and C14-18-unsatd. alkyl c	300-326-6	93925-25-8	93925258	-	-	4948														18%	-7.7	-8.0	-9.6
N,N''-methylenebis[N'-[3-(hydroxymethyl)-2,5-dioxoimidazolidi	254-372-6	39236-46-9	39236469	-	-	4949														18%	-7.7	-8.0	-9.6
2-ethylhexyl diphenyl phosphite	239-716-5	15647-08-2	15647082	-	-	4950														18%	-7.7	-8.0	-9.6
Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu	273-527-9	68988-45-4	68988454	-	-	4951														18%	-7.7	-8.0	-9.7
[tetrachloro-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]	248-573-8	27614-71-7	27614717	-	-	4952														18%	-7.7	-8.0	-9.7
Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, b	270-958-4	68512-13-0	68512130	-	-	4953														18%	-7.7	-8.0	-9.7
629-720-9	629-720-9	1219826-66-0	1219826660	-	-	4954														18%	-7.7	-8.0	-9.7
800-182-9	800-182-9	1426148-68-6	1426148686	-	-	4955														18%	-7.7	-8.0	-9.7
609-530-2	609-530-2	38172-91-7	38172917	-	-	4956														18%	-7.7	-8.0	-9.7
isodecyl pivalate	262-108-6	60209-82-7	60209827	-	-	4957														18%	-7.7	-8.0	-9.7
Reaction products of ethane-1,2-diol and 1,2-epoxybutane	695-757-2	897381-19-0	897381190	-	-	4958														18%	-7.7	-8.0	-9.7
Aluminum, benzoate C16-18-fatty acids complexes	303-385-6	94166-87-7	94166877	-	-	4959														18%	-7.7	-8.0	-9.7
Quaternary ammonium compounds, C12-18-alkylbis(hydroxyet	276-038-9	71808-53-2	71808532	-	-	4960														18%	-7.7	-8.0	-9.7
Terpenes and terpenoids, turpentine-oil, α-pinene fraction, olig	500-245-8	70750-57-1	70750571	-	-	4961														18%	-7.7	-8.0	-9.7
pentasodium pentahydrogen [[(phosphonatomethyl)imino]bis[	263-212-4	61792-09-4	61792094	-	-	4962														18%	-7.7	-8.0	-9.7
Isooctadecanoic acid, reaction products with tetraethylenepent	272-225-4	68784-17-8	68784178	-	-	4963														18%	-7.7	-8.0	-9.7
Lipase, triacylglycerol	232-619-9	9001-62-1	9001621	-	-	4964														18%	-7.7	-8.0	-9.7
Quaternary ammonium compounds, benzyl-C12-16-alkyldimetl	270-325-2	68424-85-1	68424851	-	-	4965														18%	-7.7	-8.0	-9.7
Fatty acids, C16-18 and C18-unsatd., iso-Bu esters	284-868-8	84988-79-4	84988794	-	-	4966														18%	-7.7	-8.0	-9.7
Tetra-n-butyl titanate, polymer with water	500-687-1	162303-51-7	162303517	-	-	4967														18%	-7.7	-8.0	-9.7
695-101-5	695-101-5	1275611-65-8	1275611658	-	-	4968														18%	-7.7	-8.0	-9.7
Cocoa, powd., alkalized	305-748-4	95009-22-6	95009226	-	-	4969														18%	-7.7	-8.0	-9.7
Fatty acids, C16-18, 2-hexyldecyl esters	309-832-1	101227-09-2	101227092	-	-	4970														18%	-7.7	-8.0	-9.7
Fatty acids, C6-18, 2,2-dimethyl-1,3-propanediyl esters	292-927-4	91031-27-5	91031275	-	-	4971														18%	-7.7	-8.0	-9.7
696-364-9	696-364-9	133779-11-0	133779110	-	-	4972														18%	-7.7	-8.0	-9.7
600-026-8	600-026-8	1000817-22-0	1000817220	-	-	4973														18%	-7.7	-8.0	-9.7
isopropyl isodecanoate	269-023-3	68171-33-5	68171335	-	-	4974														18%	-7.7	-8.0	-9.7
pentaerythritol tetraoleate	242-960-5	19321-40-5	19321405	-	-	4975														18%	-7.7	-8.0	-9.7
616-248-3	616-248-3	75627-31-5	75627315	-	-	4976														18%	-7.7	-8.0	-9.7
Glycerides, C14-18 mono- and di-	266-952-6	67701-33-1	67701331	-	-	4977														18%	-7.7	-8.0	-9.7
Titanium, diethylene glycol propylene glycol triethanolamine cc	272-250-0	68784-48-5	68784485	-	-	4978														18%	-7.7	-8.0	-9.7
oleic acid, compound with N-(2-aminoethyl)ethane-1,2-diamine	241-924-6	18016-43-8	18016438	-	-	4979														18%	-7.7	-8.0	-9.7
1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	219-514-3	2451-62-9	2451629	-	-	4980														18%	-7.7	-8.0	-9.7
Octadecanoic acid, 12-hydroxy-, reaction products with ethyler	309-629-8	100545-48-0	100545480	-	-	4981														18%	-7.7	-8.1	-9.7
2,3-dihydroxypropyl 12-hydroxyoctadecanoate	228-507-4	6284-43-1	6284431	-	-	4982														18%	-7.7	-8.1	-9.7
692-946-1	692-946-1	649747-80-8	649747808	-	-	4983														18%	-7.7	-8.1	-9.7
696-028-1	696-028-1	1334537-35-7	1334537357	-	-	4984														18%	-7.7	-8.1	-9.7
Reaction mass of ammonium 4-amino-3-nitrobenzenesulfonate	700-384-6	82324-60-5	82324605	-	-	4985														18%	-7.7	-8.1	-9.7
614-587-1	614-587-1	68551-92-8	68551928	-	-	4986														18%	-7.7	-8.1	-9.7
4,4'-Methylenediphenyl diisocyanate, oligomeric reaction prod	500-297-1	109331-54-6	109331546	-	-	4987														18%	-7.7	-8.1	-9.7
Mannanase, endo-1,4-β-	253-446-5	37288-54-3	37288543	-	-	4988														18%	-7.7	-8.1	-9.7
Soybean oil, epoxidized, reaction products with methanol	287-837-7	85586-35-2	85586352	-	-	4989														18%	-7.8	-8.1	-9.7
Fatty acids, tallow, calcium salts	265-228-7	64755-01-7	64755017	-	-	4990														18%	-7.8	-8.1	-9.7
sodium glucoheptonate	250-480-2	31138-65-5	31138655	-	-	4991														18%	-7.8	-8.1	-9.7
Phosphoric acid, butyl ester	235-826-2	12788-93-1	12788931	-	-	4992														18%	-7.8	-8.1	-9.7
608-744-3	608-744-3	32472-85-8	32472858	-	-	4993														18%	-7.8	-8.1	-9.7
Glycerides, mixed C8-10 and succinyl	294-620-0	91744-56-8	91744568	-	-	4994														18%	-7.8	-8.1	-9.7
614-339-2	614-339-2	68154-62-1	68154621	-	-	4995														18%	-7.8	-8.1	-9.7
Tall oil, potassium salt	271-968-1	68647-71-2	68647712	-	-	4996														18%	-7.8	-8.1	-9.7
Fatty acids, C14-18 and C18-unsatd., branched and linear, ester	284-957-1	85005-25-0	85005250	-	-	4997														18%	-7.8	-8.1	-9.7
Resin acids and Rosin acids, esters with ethylene glycol	270-986-7	68512-65-2	68512652	-	-	4998														18%	-7.8	-8.1	-9.7
Sorbitan, isooctadecanoate	276-171-2	71902-01-7	71902017	-	-	4999														18%	-7.8	-8.1	-9.7
610-559-8	610-559-8	50658-23-6	50658236	-	-	5000														18%	-7.8	-8.1	-9.7
Phosphoric acid, hexyl ester	270-935-9	68511-03-5	68511035	-	-	5001														18%	-7.8	-8.1	-9.7
monoethanolamine oleate	218-878-0	2272-11-9	2272119	-	-	5002														18%	-7.8	-8.1	-9.7
Heptanoic acid, ester with 2-ethyl-2-(hydroxymethyl)-1,3-propa	267-029-0	67762-64-5	67762645	-	-	5003														18%	-7.8	-8.1	-9.7
800-029-6	800-029-6	1290049-56-7	1290049567	-	-	5004														18%	-7.8	-8.1	-9.7
Amines, C36-alkylenedi-	273-282-8	68955-56-6	68955566	-	-	5005														18%	-7.8	-8.1	-9.7
1,2,3-Propanetriol, glycidyl ethers	292-011-4	90529-77-4	90529774	-	-	5006														18%	-7.8	-8.1	-9.7

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Quaternary ammonium compounds, bis(hydrogenated tallow a	263-090-2	61789-80-8	61789808	-	-	5007														18%	-7.8	-8.1	-9.7
3-(2-dodecenyl)succinic anhydride	243-296-9	19780-11-1	19780111	-	-	5008														18%	-7.8	-8.1	-9.8
Sorbitan, octanoate (2:3)	295-118-4	91844-53-0	91844530	-	-	5009														18%	-7.8	-8.1	-9.8
606-712-3	606-712-3	211450-54-3	211450543	-	-	5010														18%	-7.8	-8.1	-9.8
608-035-9	608-035-9	27014-42-2	27014422	-	-	5011														18%	-7.8	-8.1	-9.8
1,3-Propanediamine, N-[3-(tridecyloxy)propyl]-, branched	270-851-2	68479-04-9	68479049	-	-	5012														18%	-7.8	-8.1	-9.8
Fatty acids, C8-10, zinc salts	293-048-9	91051-00-2	91051002	-	-	5013														18%	-7.8	-8.1	-9.8
mono- and di-esterification products of propane-1,2,3-triol anc	800-149-9	1410795-90-2	1410795902	-	-	5014														18%	-7.8	-8.1	-9.8
Resin acids and Rosin acids, hydrogenated, Me esters	232-476-2	8050-15-5	8050155	-	-	5015														18%	-7.8	-8.1	-9.8
1-[1,3-bis(hydroxymethyl)-2,5-dioxoimidazolidin-4-yl]-1,3-bis(h	278-928-2	78491-02-8	78491028	-	-	5016														18%	-7.8	-8.1	-9.8
806-508-6	806-508-6	1419212-77-3	1419212773	-	-	5017														18%	-7.8	-8.1	-9.8
tetradonium bromide	214-291-9	1119-97-7	1119977	-	-	5018														18%	-7.8	-8.1	-9.8
609-542-8	609-542-8	383178-66-3	383178663	-	-	5019														18%	-7.8	-8.1	-9.8
Tar bases, coal, picoline fraction	295-548-2	92062-33-4	92062334	-	-	5020														18%	-7.8	-8.1	-9.8
800-760-0	800-760-0	68139-89-9	68139899	-	-	5021														18%	-7.8	-8.1	-9.8
Phenol, heptyl derivs.	276-743-1	72624-02-3	72624023	-	-	5022														18%	-7.8	-8.1	-9.8
2-Butenedioic acid (E)-, di-C8-18-alkyl esters	271-880-3	68610-90-2	68610902	-	-	5023														18%	-7.8	-8.1	-9.8
1,3,5-Triazine-2,4,6-triamine, deammoniated	272-034-6	68649-66-1	68649661	-	-	5024														18%	-7.8	-8.1	-9.8
Formaldehyde, reaction products with ethylenediamine	281-928-5	84066-92-2	84066922	-	-	5025														18%	-7.8	-8.1	-9.8
Fatty acids, C16-18, tetraesters with 3,3'-oxybis[1,2-propanedi	293-026-9	91050-80-5	91050805	-	-	5026														18%	-7.8	-8.1	-9.8
Fatty acids, tall-oil, iron salts	263-009-0	61788-81-6	61788816	-	-	5027														18%	-7.8	-8.1	-9.8
609-271-5	609-271-5	36609-29-7	36609297	-	-	5028														18%	-7.8	-8.1	-9.8
Isooctadecanoic acid, mono- and diesters with glycerol	306-657-2	97358-80-0	97358800	-	-	5029														18%	-7.8	-8.1	-9.8
3-(methacryloylamino)-N,N-dimethylpropan-1-aminium 4-(C10	688-489-2	1024700-50-2	1024700502	-	-	5030														18%	-7.8	-8.1	-9.8
611-591-5	611-591-5	57903-73-8	57903738	-	-	5031														18%	-7.8	-8.1	-9.8
Fatty acids, C8-10, mixed esters with adipic acid and trimethylo	306-085-3	95912-89-3	95912893	-	-	5032														18%	-7.8	-8.2	-9.8
Decanoic acid, mixed esters with neopentyl glycol and octanoic	274-764-0	70693-32-2	70693322	-	-	5033														18%	-7.8	-8.2	-9.8
benzene-1,2,4,5-tetracarboxylic acid, compound with 4,5-dihyc	259-224-4	54553-90-1	54553901	-	-	5034														18%	-7.9	-8.2	-9.8
Propanenitrile, 3,3'-iminobis-, N-tallow alkyl derivs.	270-194-1	68412-52-2	68412522	-	-	5035														18%	-7.9	-8.2	-9.8
1-(tert-dodecylthio)propan-2-ol	266-582-5	67124-09-8	67124098	-	-	5036														18%	-7.9	-8.2	-9.8
613-868-6	613-868-6	65997-12-8	65997128	-	-	5037														18%	-7.9	-8.2	-9.8
2-octyldodecyl isooctadecanoate	298-361-4	93803-87-3	93803873	-	-	5038														18%	-7.9	-8.2	-9.8
Alcohols, C8-10, ethoxylated, sulfates, ammonium salts	500-233-2	68891-29-2	68891292	-	-	5039														18%	-7.9	-8.2	-9.8
Glycerides, C8-10 mono- and di-	287-488-0	85536-07-8	85536078	-	-	5040														18%	-7.9	-8.2	-9.8
2-Hexyldecan-1-ol, ethoxylated	500-116-6	52609-19-5	52609195	-	-	5041														18%	-7.9	-8.2	-9.8
613-584-2	613-584-2	64401-02-1	64401021	-	-	5042														18%	-7.9	-8.2	-9.9
2,4,7,9-Tetramethyldec-5-yne-4,7-diol, ethoxylated	500-022-5	9014-85-1	9014851	-	-	5043														18%	-7.9	-8.2	-9.9
Rape oil, reaction products with diethanolamine	269-125-8	68187-80-4	68187804	-	-	5044														18%	-7.9	-8.2	-9.9
638-747-5	638-747-5	1228186-17-1	1228186171	-	-	5045														18%	-7.9	-8.2	-9.9
604-714-9	604-714-9	149968-48-9	149968489	-	-	5046														18%	-7.9	-8.2	-9.9
oleic acid, monoester with oxybis(propanediol)	256-367-4	49553-76-6	49553766	-	-	5047														18%	-7.9	-8.2	-9.9
zinc bis[O-(2-ethylhexyl)] bis[O-(isobutyl)] bis(dithiophosphate)	247-810-2	26566-95-0	26566950	-	-	5048														18%	-7.9	-8.2	-9.9
Fatty acids, C18-unsatd., dimers, oligomeric reaction products	500-289-8	103758-98-1	103758981	-	-	5049														18%	-7.9	-8.2	-9.9
604-617-1	604-617-1	147993-66-6	147993666	-	-	5050														18%	-7.9	-8.2	-9.9
Poly(oxy-1,2-ethanediyl),α-hydro-ω-hydroxy- Ethane-1,2-diol, e	500-038-2	25322-68-3	25322683	-	-	5051														18%	-7.9	-8.2	-9.9
dioctyltin dilaurate	222-883-3	3648-18-8	3648188	-	-	5052														18%	-7.9	-8.2	-9.9
3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-3-en-2-on	265-450-4	65113-95-3	65113953	-	-	5053														18%	-7.9	-8.2	-9.9
Hydrocarbons, C12-30, olefin-rich, ethylene polymn. by-produc	272-762-4	68911-05-7	68911057	-	-	5054														18%	-7.9	-8.2	-9.9
DL-lysine monohydrochloride	200-739-0	70-53-1	70531	-	-	5055														18%	-7.9	-8.2	-9.9
800-310-3	800-310-3	78683-74-6	78683746	-	-	5056														18%	-7.9	-8.2	-9.9
Alcohols, lanolin, distn. residues	292-441-2	90622-40-5	90622405	-	-	5057														18%	-7.9	-8.2	-9.9
806-509-1	806-509-1	1393571-42-0	1393571420	-	-	5058														18%	-7.9	-8.2	-9.9
Polysulfides, di-tert-nonyl	270-336-2	68425-16-1	68425161	-	-	5059														18%	-7.9	-8.2	-9.9
Phosphoric acid, mixed esters with Bu alc. and ethylene glycol	284-716-0	84962-20-9	84962209	-	-	5060														18%	-7.9	-8.2	-9.9
2,3-Epoxypropyl neodecanoate, oligomeric reaction products w	500-281-4	98362-33-5	98362335	-	-	5061														18%	-7.9	-8.2	-9.9
Glycerides, C14-18 and C16-18-unsatd. mono-, di- and tri-	293-187-5	91052-28-7	91052287	-	-	5062														18%	-7.9	-8.2	-9.9
Benzenamine, reaction products with aniline hydrochloride anc	309-913-1	101357-16-8	101357168	-	-	5063														18%	-7.9	-8.3	-9.9
4,4'-Isopropylidenediphenol, oligomeric reaction products with	500-652-0	161308-12-9	161308129	-	-	5064														18%	-7.9	-8.3	-9.9
600-028-9	600-028-9	1001254-87-0	1001254870	-	-	5065														18%	-8.0	-8.3	-9.9
Fatty acids, lanolin, iso-Pr esters	264-119-1	63393-93-1	63393931	-	-	5066														18%	-8.0	-8.3	-9.9
sorbitan tristearate	247-891-4	26658-19-5	26658195	-	-	5067														18%	-8.0	-8.3	-9.9
Formaldehyde, reaction products with m-phenylenediamine, sc	274-986-8	70892-34-1	70892341	-	-	5068														18%	-8.0	-8.3	-9.9
Resin acids and Rosin acids, maleated, calcium salts	294-402-5	91722-01-9	91722019	-	-	5069														18%	-8.0	-8.3	-9.9
Quaternary ammonium compounds, (hydrogenated tallow alky	263-005-9	61788-78-1	61788781	-	-	5070														18%	-8.0	-8.3	-9.9
Butanedioic acid, sulfo-, monoesters with lanolin alcs., disodiur	290-844-8	90268-43-2	90268432	-	-	5071														18%	-8.0	-8.3	-9.9
Butanedioic acid, sulfo-, 4-[2-[(2-hydroxyethyl)amino]ethyl] est	308-072-8	97862-28-7	97862287	-	-	5072														18%	-8.0	-8.3	-9.9
Fatty acids, C14-18 and C16-18-unsatd., mixed esters with cast	295-653-3	92113-48-9	92113489	-	-	5073														18%	-8.0	-8.3	-9.9
800-906-3	800-906-3	1402434-48-3	1402434483	-	-	5074														18%	-8.0	-8.3	-9.9
Phosphoric acid, mono- and di-C12-14-alkyl esters	308-020-4	97808-97-4	97808974	-	-	5075														18%	-8.0	-8.3	-9.9
800-362-7	800-362-7	1307863-78-0	1307863780	-	-	5076														18%	-8.0	-8.3	-9.9
9-Octadecenoic acid (Z)-, isooctyl ester, reaction products with	306-111-3	96152-40-8	96152408	-	-	5077														18%	-8.0	-8.3	-9.9
Fatty acids, tall-oil, magnesium salts	266-942-1	67701-23-9	67701239	-	-	5078														18%	-8.0	-8.3	-9.9
2-Propenoic acid, 2-methyl-, 2-hydroxyethyl ester, phosphate	258-053-2	52628-03-2	52628032	-	-	5079														18%	-8.0	-8.3	-9.9
2-Butenedioic acid (E)-, di-C16-18-alkyl esters	272-944-3	68921-52-8	68921528	-	-	5080														18%	-8.0	-8.3	-9.9
3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-ol	267-140-4	67801-20-1	67801201	-	-	5081														18%	-8.0	-8.3	-10.0

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Peptones, beef	293-426-3	91079-38-8	91079388	-	-	5082														18%	-8.0	-8.3	-10.0
menthane, monohydroperoxy derivative	247-987-6	26762-92-5	26762925	-	-	5083														18%	-8.0	-8.3	-10.0
695-121-4	695-121-4	1178870-70-6	1178870706	-	-	5084														18%	-8.0	-8.3	-10.0
800-767-9	800-767-9	1424148-94-6	1424148946	-	-	5085														18%	-8.0	-8.3	-10.0
zinc bis[bis(dodecylphenyl)] bis(dithiophosphate)	259-048-8	54261-67-5	54261675	-	-	5086														18%	-8.0	-8.3	-10.0
Sulfonium compounds, C11-14-alkylbis(hydroxyethyl), 2-hydro	278-855-6	78169-20-7	78169207	-	-	5087														18%	-8.0	-8.3	-10.0
dihydro-3-(tripropenyl)furan-2,5-dione	295-556-6	92077-08-2	92077082	-	-	5088														18%	-8.0	-8.3	-10.0
fatty acids, C16-18 and C18-unsatd., isooctyl esters, epoxidized	307-159-8	97553-05-4	97553054	-	-	5089														18%	-8.0	-8.3	-10.0
Hexafluoropropene, oxidized, oligomers, reduced, fluorinated	500-537-5	161075-00-9	161075009	-	-	5090														18%	-8.0	-8.3	-10.0
605-658-8	605-658-8	173011-06-8	173011068	-	-	5091														18%	-8.0	-8.3	-10.0
3-methyl-5-phenylpentanol	259-461-3	55066-48-3	55066483	-	-	5092														18%	-8.0	-8.3	-10.0
isodecyl acrylate	215-542-5	1330-61-6	1330616	-	-	5093														18%	-8.0	-8.4	-10.0
604-250-7	604-250-7	141773-73-1	141773731	-	-	5094														18%	-8.1	-8.4	-10.0
(octahydro-4,7-methano-1H-indenediyl)bis(methylene) diacryla	255-901-3	42594-17-2	42594172	-	-	5095														18%	-8.1	-8.4	-10.0
Rape oil, sulfated, sodium salt	281-978-8	84082-30-4	84082304	-	-	5096														18%	-8.1	-8.4	-10.0
Amines, N-C16-22-alkyltrimethylenedi-	292-564-1	90640-45-2	90640452	-	-	5097														18%	-8.1	-8.4	-10.0
Dodecan-1-ol, ethoxylated	500-002-6	9002-92-0	9002920	-	-	5098														18%	-8.1	-8.4	-10.0
[N,N,N',N',N'',N''-hexaethyl-29H,31H-phthalocyaninetrimethyla	249-125-4	28654-73-1	28654731	-	-	5099														18%	-8.1	-8.4	-10.0
N,N-dibutyloleamide	227-410-4	5831-80-1	5831801	-	-	5100														18%	-8.1	-8.4	-10.0
614-482-0	614-482-0	68439-46-3	68439463	-	-	5101														18%	-8.1	-8.4	-10.0
800-153-0	800-153-0	1313206-64-2	1313206642	-	-	5102														18%	-8.1	-8.4	-10.0
3-(methacryloylamino)-N,N,N-trimethylpropan-1-aminium 4-(C	688-159-8	1024699-81-7	1024699817	-	-	5103														18%	-8.1	-8.4	-10.0
695-088-6	695-088-6	135458-18-3	135458183	-	-	5104														18%	-8.1	-8.4	-10.0
613-645-3	613-645-3	646505-36-4	646505364	-	-	5105														18%	-8.1	-8.4	-10.0
Aluminum, hydrobis(2-methylpropyl)-, reaction products with i	274-261-6	70024-64-5	70024645	-	-	5106														18%	-8.1	-8.4	-10.0
di(isooctadecanoic) acid, diester with oxydi(propanediol)	267-821-6	67938-21-0	67938210	-	-	5107														18%	-8.1	-8.4	-10.0
696-481-5	696-481-5	1219826-47-7	1219826477	-	-	5108														18%	-8.1	-8.4	-10.0
isooctyl 3-mercaptopropionate	250-157-6	30374-01-7	30374017	-	-	5109														18%	-8.1	-8.4	-10.0
1,1,3,3-tetramethylbutyl peroxyneodecanoate	257-077-0	51240-95-0	51240950	-	-	5110														18%	-8.1	-8.4	-10.0
2,2-bis(hydroxymethyl)-1,3-propanediyl dioleate	246-665-2	25151-96-6	25151966	-	-	5111														18%	-8.1	-8.4	-10.1
600-687-2	600-687-2	105839-18-7	105839187	-	-	5112														18%	-8.1	-8.4	-10.1
619-721-2	619-721-2	1079258-99-3	1079258993	-	-	5113														18%	-8.1	-8.4	-10.1
2,6-dimethylindan-1-amine	937-760-6	1225478-65-8	1225478658	-	-	5114														18%	-8.1	-8.4	-10.1
Reaction mass of ammonium 2-amino-4-[(4-amino-6-chloro-1,:	937-657-6	1362924-06-8	1362924068	-	-	5115														18%	-8.1	-8.4	-10.1
800-766-3	800-766-3	1424148-97-9	1424148979	-	-	5116														18%	-8.1	-8.4	-10.1
800-765-8	800-765-8	1424149-03-0	1424149030	-	-	5117														18%	-8.1	-8.4	-10.1
Reaction mass of dimethyl 2,2,4-trimethylhexanedioate and dir	700-087-1	201872-72-2	201872722	-	-	5118														18%	-8.1	-8.4	-10.1
607-104-0	607-104-0	225375-65-5	225375655	-	-	5119														18%	-8.1	-8.4	-10.1
O,O-bis(methylphenyl) hydrogen dithiophosphate	248-273-7	27157-94-4	27157944	-	-	5120														18%	-8.1	-8.4	-10.1
nonene	248-339-5	27215-95-8	27215958	-	-	5121														18%	-8.1	-8.4	-10.1
(1R*,6S*)-6-(ethoxycarbonyl)-N,N-dimethyl-6-phenylcyclohex-2	700-689-4	41524-32-7	41524327	-	-	5122														18%	-8.1	-8.4	-10.1
3,7-dimethylnona-2,6-dienenitrile	263-214-5	61792-11-8	61792118	-	-	5123														18%	-8.1	-8.4	-10.1
Extract oils (coal), tar base	266-020-9	65996-86-3	65996863	-	-	5124														18%	-8.1	-8.4	-10.1
Butanal, reaction products with aniline	270-109-8	68411-20-1	68411201	-	-	5125														18%	-8.1	-8.4	-10.1
Gases (petroleum), acetylene manuf. off	270-745-6	68477-64-5	68477645	-	-	5126														18%	-8.1	-8.4	-10.1
Urea, reaction products with formaldehyde	271-898-1	68611-64-3	68611643	-	-	5127														18%	-8.1	-8.4	-10.1
Propanenitrile, 3-amino-, N-coco alkyl derivs.	272-244-8	68784-40-7	68784407	-	-	5128														18%	-8.1	-8.4	-10.1
6,10-dimethylundeca-5,9-dien-2-one	211-711-2	689-67-8	689678	-	-	5129														18%	-8.1	-8.4	-10.1
Coconut oil, hydrogenated	284-283-8	84836-98-6	84836986	-	-	5130														18%	-8.1	-8.4	-10.1
distillates (coal tar), upper, fluorene-rich	284-900-0	84989-11-7	84989117	-	-	5131														18%	-8.1	-8.4	-10.1
Amines, N-(3-aminopropyl)-N-tallow alkyltrimethylenedi-	288-048-0	85632-63-9	85632639	-	-	5132														18%	-8.1	-8.4	-10.1
isohexadecene	288-853-7	85909-49-5	85909495	-	-	5133														18%	-8.1	-8.4	-10.1
Alkyl iodides, C6-18, perfluoro	292-474-2	90622-71-2	90622712	-	-	5134														18%	-8.1	-8.4	-10.1
Fatty acids, C18-22	292-772-2	90990-11-7	90990117	-	-	5135														18%	-8.1	-8.4	-10.1
dodecahydro-3a,6,6,9a-tetramethylnaphtho[2,1-b]furan	223-118-6	3738-00-9	3738009	-	-	5136														18%	-8.1	-8.4	-10.1
Fatty acids, coco, isotridecyl esters	292-997-6	91031-91-3	91031913	-	-	5137														18%	-8.1	-8.4	-10.1
607-255-2	607-255-2	236391-76-7	236391767	-	-	5138														18%	-8.1	-8.4	-10.1
613-848-7	613-848-7	65870-94-2	65870942	-	-	5139														18%	-8.1	-8.4	-10.1
Glycerides, C12-18 mono- and di-	293-209-3	91052-49-2	91052492	-	-	5140														18%	-8.1	-8.4	-10.1
614-255-6	614-255-6	68071-07-8	68071078	-	-	5141														18%	-8.1	-8.4	-10.1
695-977-9	695-977-9	1309955-79-0	1309955790	-	-	5142														18%	-8.1	-8.4	-10.1
614-452-7	614-452-7	68410-23-1	68410231	-	-	5143														18%	-8.1	-8.4	-10.1
Fatty acids, C14-18 and C16-18-unsatd., isotridecyl esters	285-541-2	85116-88-7	85116887	-	-	5144														18%	-8.1	-8.4	-10.1
Alkenes, C24-28 α-	300-203-7	93924-11-9	93924119	-	-	5145														18%	-8.1	-8.4	-10.1
Lysozyme (chicken egg white)	235-747-3	12650-88-3	12650883	-	-	5146														18%	-8.1	-8.4	-10.1
Alcohols, C16-18, ethoxylated, phosphates	500-295-0	106233-09-4	106233094	-	-	5147														18%	-8.1	-8.4	-10.1
2-Butenedioic acid (E)-, di-C18-22-alkyl esters	272-945-9	68921-53-9	68921539	-	-	5148														18%	-8.1	-8.4	-10.1
Fatty acids, tall-oil, reaction products with boric acid (H3BO3) a	294-785-9	91770-03-5	91770035	-	-	5149														18%	-8.1	-8.4	-10.1
Fatty acids, C8-10, triesters with trimethylolpropane	293-036-3	91050-89-4	91050894	-	-	5150														18%	-8.1	-8.4	-10.1
Amines, tri-C8-10-alkyl	272-347-8	68814-95-9	68814959	-	-	5151														18%	-8.1	-8.4	-10.1
Phosphoric acid, isononyl ester	284-851-5	84988-61-4	84988614	-	-	5152														18%	-8.1	-8.4	-10.1
627-071-6	627-071-6	1233873-37-4	1233873374	-	-	5153														18%	-8.1	-8.5	-10.1
Hydrochloric acid, reaction products with aniline and nitrobenz	291-454-0	90411-76-0	90411760	-	-	5154														18%	-8.2	-8.5	-10.1
Decanoic acid, mixed esters with heptanoic acid, octanoic acid,	275-118-0	71010-76-9	71010769	-	-	5155														18%	-8.2	-8.5	-10.1
608-711-3	608-711-3	32167-31-0	32167310	-	-	5156														18%	-8.2	-8.5	-10.1

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Tall oil, compd. with ethanolamine	268-069-1	68002-54-0	68002540	-	-	5157														18%	-8.2	-8.5	-10.1
Propylidynetrimethanol, ethoxylated, esters with acrylic acid, re	500-425-6	159034-91-0	159034910	-	-	5158														18%	-8.2	-8.5	-10.1
Naphthenic acids, potassium salts	266-120-2	66072-08-0	66072080	-	-	5159														18%	-8.2	-8.5	-10.1
Tall oil, compd. with diethanolamine	268-452-3	68092-28-4	68092284	-	-	5160														18%	-8.2	-8.5	-10.1
Alcohols, C12-15, ethoxylated	500-195-7	68131-39-5	68131395	-	-	5161														18%	-8.2	-8.5	-10.1
614-557-8	614-557-8	68515-81-1	68515811	-	-	5162														18%	-8.2	-8.5	-10.1
[N,N,N',N',N'',N''-hexaethyl-29H,31H-phthalocyaninetrimethyla	278-150-3	75247-18-6	75247186	-	-	5163														18%	-8.2	-8.5	-10.1
630-459-8	630-459-8	1225197-81-8	1225197818	-	-	5164														18%	-8.2	-8.5	-10.1
Cyclohexane, oxidized, non-volatile residue	270-147-5	68411-76-7	68411767	-	-	5165														18%	-8.2	-8.5	-10.2
806-914-3	806-914-3	1499182-59-0	1499182590	-	-	5166														18%	-8.2	-8.5	-10.2
Asphalt, sulfonated, sodium salt	269-212-0	68201-32-1	68201321	-	-	5167														18%	-8.2	-8.5	-10.2
N-[9-(dichloromethylidene)-1,2,3,4-tetrahydro-1,4-methanona	691-719-4	1072957-71-1	1072957711	-	-	5168														18%	-8.2	-8.5	-10.2
methyl 3,5,5-trimethylhexanoate	807-032-1	71500-39-5	71500395	-	-	5169														18%	-8.2	-8.5	-10.2
Sorbitan monostearate, ethoxylated	500-020-4	9005-67-8	9005678	-	-	5170														18%	-8.2	-8.5	-10.2
Myristica fragrans, ext.	282-013-3	84082-68-8	84082688	-	-	5171														18%	-8.3	-8.6	-10.2
triisononanoic acid, triester with 2,2'-[oxybis(methylene)]bis[2-	270-560-0	68443-84-5	68443845	-	-	5172														18%	-8.3	-8.6	-10.2
Benzoic acid, 2-hydroxy-, mono-C>13-alkyl derivs., calcium salts	281-018-8	83846-43-9	83846439	-	-	5173														18%	-8.3	-8.6	-10.2
Reaction mass of bis[2,4-bis(2-methylbutan-2-yl)phenyl] 4-(2-m	700-485-5	939402-02-5	939402025	-	-	5174														18%	-8.3	-8.6	-10.2
Phosphoric acid, mono- and di-C6-10-alkyl esters	269-616-7	68307-94-8	68307948	-	-	5175														18%	-8.3	-8.6	-10.2
mercaptoacetic acid, monoester with propane-1,2,3-triol	250-264-8	30618-84-9	30618849	-	-	5176														18%	-8.3	-8.6	-10.3
800-770-5	800-770-5	1424148-99-1	1424148991	-	-	5177														18%	-8.3	-8.6	-10.3
607-234-8	607-234-8	234446-82-3	234446823	-	-	5178														18%	-8.3	-8.6	-10.3
Resin acids and Rosin acids, hydrogenated, esters with triethyle	271-996-4	68648-53-3	68648533	-	-	5179														18%	-8.3	-8.6	-10.3
605-694-4	605-694-4	173832-46-7	173832467	-	-	5180														18%	-8.3	-8.7	-10.3
Ammonium difluoro{[2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1	682-238-0	1190931-27-1	1190931271	-	-	5181														18%	-8.3	-8.7	-10.3
pentan-2-one O-(4,10-dimethyl-7-vinyl-6,8-dioxa-5,9-diaza-7-si	700-810-0	58190-62-8	58190628	-	-	5182														18%	-8.4	-8.7	-10.3
Octadecanoic acid, reaction products with diethylenetriamine a	284-698-4	84962-05-0	84962050	-	-	5183														18%	-8.4	-8.7	-10.3
5-isopropylimidazolidine-2,4-dione	634-107-4	16935-34-5	16935345	-	-	5184														18%	-8.4	-8.7	-10.4
5-methyl-2-(1-methylvinyl)cyclohexan-1-ol	232-102-8	7786-67-6	7786676	-	-	5185														18%	-8.4	-8.7	-10.4
diisotridecyl 3,3'-[(dibutylstannylene)bis(thio)]dipropionate	284-461-5	84896-44-6	84896446	-	-	5186														18%	-8.4	-8.7	-10.4
Heptadecanol, branched and linear	291-378-8	90388-00-4	90388004	-	-	5187														18%	-8.4	-8.7	-10.4
2-Butene, chlorinated, epoxidized, distn. residues	304-783-2	94279-39-7	94279397	-	-	5188														18%	-8.4	-8.7	-10.4
1-Propene, 2-methyl-, chlorinated, epoxidized, distn. residues	304-801-9	94279-55-7	94279557	-	-	5189														18%	-8.4	-8.7	-10.4
2-ethyl-2-[[(1-oxoisooctadecyl)oxy]methyl]-1,3-propanediyl bis	271-347-5	68541-50-4	68541504	-	-	5190														18%	-8.4	-8.7	-10.4
Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo	272-732-0	68910-13-4	68910134	-	-	5191														18%	-8.6	-8.9	-10.5
Tar bases, coal, lutidine fraction	293-766-2	91082-52-9	91082529	-	-	5192														18%	-8.6	-8.9	-10.5
tris(dodecyl and/or octyl) benzene-1,2,4-tricarboxylate	700-342-7	1163775-81-2	1163775812	-	-	5193														18%	-8.6	-8.9	-10.5
dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione	254-100-6	38720-66-0	38720660	-	-	5194														18%	-8.6	-8.9	-10.6
reaction products of zinc oxide and glycerol	700-107-9	87189-25-1	87189251	-	-	5195														18%	-8.6	-8.9	-10.6
Esterification product of castor oil and tetrahydromethyl-1,3-is	700-064-6	1059667-42-3	1059667423	-	-	5196														18%	-8.6	-8.9	-10.6
Coupling reaction products of diazotized 2-amino-6-[(2-sulfoetl	700-470-3	1198102-85-0	1198102850	-	-	5197														18%	-8.7	-9.0	-10.6
Resin acids and Rosin acids, reaction products with formaldehy	696-130-6	1364681-45-7	1364681457	-	-	5198														18%	-8.7	-9.0	-10.7
Ethyl-2-cyano-2-ethyl-3-methylhexanoate	700-063-0	100453-11-0	100453110	-	-	5199														18%	-8.8	-9.1	-10.8
D-Glucopyranose, oligomers, branched and linear C9-11-alkyl g	500-394-9	157707-87-4	157707874	-	-	5200														18%	-8.8	-9.1	-10.8
Resin acids and Rosin acids, Me esters	269-035-9	68186-14-1	68186141	-	-	5201														18%	-8.8	-9.2	-10.8
Potassium difluoro{[2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,	682-240-1	1190931-39-5	1190931395	-	-	5202														18%	-8.9	-9.2	-10.9
Reaction products of 2,2'-oxydiethanol and 3-(triethoxysilyl)prc	688-124-7	152261-43-3	152261433	-	-	5203														18%	-8.9	-9.2	-10.9
7,7,9(or 7,9,9)-trimethyl-4,13-dioxo-3,14-dioxa-5,12-diazahexa	276-957-5	72869-86-4	72869864	-	-	5204														18%	-8.9	-9.2	-10.9
dibutyltin bis(2-ethylhexanoate)	220-481-2	2781-10-4	2781104	-	-	5205														18%	-9.0	-9.3	-10.9
Reaction products of diazotized 5-({4-[(3-amino-4-sulfophenyl)	619-894-4	958872-41-8	958872418	-	-	5206														18%	-9.0	-9.3	-11.0
Difluoro{[2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan	682-239-6	1190931-41-9	1190931419	-	-	5207														18%	-9.0	-9.3	-11.0
Silicic acid (H4SiO4), tetraethyl ester, reaction products with bis	300-344-4	93925-42-9	93925429	-	-	5208														18%	-9.1	-9.4	-11.0
D-Glucopyranose, oligomeric, C10-16 (even numbered) alkyl gly	664-492-4	742087-49-6	742087496	-	-	5209														18%	-9.1	-9.4	-11.0
606-441-0	606-441-0	201305-16-0	201305160	-	-	5210														18%	-9.1	-9.4	-11.0
Esterification products of 2,2'-(oxydimethanediyl)bis[2-(hydrox	700-325-4	1149346-12-2	1149346122	-	-	5211														18%	-9.1	-9.4	-11.1
Reaction mass of (2R,2'R)-2'-methylspiro[4-azoniabicyclo[2.2.2]	696-667-6	1292815-90-7	1292815907	-	-	5212														18%	-9.1	-9.4	-11.1
3-(6-chloro-5-fluoropyrimidin-4-yl)-2-(2,4-difluorophenyl)-1-(1H	639-694-0	188416-20-8	188416208	-	-	5213														18%	-9.1	-9.4	-11.1
Tetradecan- l-ol, ethoxylated	500-059-7	27306-79-2	27306792	-	-	5214														18%	-9.1	-9.4	-11.1
1-Methoxy-3-pentadecylbenzene-[29H,31H-phthalocyaninato(2	700-057-8	350600-52-1	350600521	-	-	5215														18%	-9.1	-9.4	-11.1
D-Glucopyranose, oligomeric, decyl octyl glucosides, phosphinic	664-495-0	740817-98-5	740817985	-	-	5216														18%	-9.1	-9.4	-11.1
619-566-0	619-566-0	848301-65-5	848301655	-	-	5217														18%	-9.1	-9.4	-11.1
619-567-6	619-567-6	848301-66-6	848301666	-	-	5218														18%	-9.1	-9.4	-11.1
619-568-1	619-568-1	848301-67-7	848301677	-	-	5219														18%	-9.1	-9.4	-11.1
Reaction mass of abieta-8,11,13-trien-18-yl [(5-{[(abieta-8,11,1	700-056-2	934985-96-3	934985963	-	-	5220														18%	-9.1	-9.4	-11.1
Esterification product of polypropylene glycol ether with glycer	700-332-2	935442-45-8	935442458	-	-	5221														18%	-9.1	-9.4	-11.1
Reaction products of Hydrogenated C18-unsaturated fatty acid	700-271-1	943862-64-4	943862644	-	-	5222														18%	-9.1	-9.4	-11.1
Ethyl 3-(2,4-dimethyl-1,3-dioxolan-2-yl)propanoate	700-636-5	5413-49-0	5413490	-	-	5223														18%	-9.1	-9.4	-11.1
Ethyl 3-[4-(hydroxymethyl)-2-methyl-1,3-dioxolan-2-yl]propanc	700-637-0	902272-78-0	902272780	-	-	5224														18%	-9.1	-9.4	-11.1
Reaction products of chlorosulfonated reaction products of cop	696-533-7	1025071-45-7	1025071457	-	-	5225														18%	-9.1	-9.4	-11.1
5',5'''-((phenylmethanediyl)bis[(2-methoxybenzene-4,1-diyl)dia	700-136-7	1062263-18-6	1062263186	-	-	5226														18%	-9.1	-9.4	-11.1
1,1'-ethan-1,2-diylbisbenzene, brominated	700-158-7	1092834-40-6	1092834406	-	-	5227														18%	-9.1	-9.4	-11.1
700-772-5	700-772-5	1190961-28-4	1190961284	-	-	5228														18%	-9.1	-9.4	-11.1
hydroxylamines, di-C16-18 (even numbered) alkyl	801-599-9	1374859-51-4	1374859514	-	-	5229														18%	-9.1	-9.4	-11.1
esterification products of castor oil and polyphosphoric acids	614-406-6	68308-61-2	68308612	-	-	5230														18%	-9.1	-9.4	-11.1
Reaction products of racemic lactic acid, partially neutralized w	700-937-1	1312021-45-6	1312021456	-	-	5231														18%	-9.1	-9.4	-11.1

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
3-(C6-16, (even numbered) and C16 unsaturated alkyl)-4-(C7-1	700-132-5	863782-35-8	863782358	-	-	5232														18%	-9.1	-9.4	-11.1
Coupling reaction products of 3,3'-dichlorobiphenyl-4,4'-bis(dia	700-452-5	1032192-65-6	1032192656	-	-	5233														18%	-9.1	-9.5	-11.1
Coupling reaction products of 3,3'-dichlorobiphenyl-4,4'-bis(dia	700-448-3	1032192-78-1	1032192781	-	-	5234														18%	-9.1	-9.5	-11.1
tris[2-(4,4-dimethylpentan-2-yl)-5,7,7-trimethyloctyl] 2-hydrox	700-590-6	56727-25-4	56727254	-	-	5235														18%	-9.1	-9.5	-11.1
4,4'-methanediylbis(2,6-dimethylcyclohexanamine)	634-657-5	65962-45-0	65962450	-	-	5236														18%	-9.1	-9.5	-11.1
C13-(branched)-alkyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)prop	700-397-7	847488-62-4	847488624	-	-	5237														18%	-9.1	-9.5	-11.1
3-[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]propane-1,2-diol	289-296-2	87061-04-9	87061049	-	-	5238														18%	-9.1	-9.5	-11.1
benzene-1,2,4,5-tetracarboxylic acid, compound with 4,5-dihyc	259-226-5	54553-91-2	54553912	-	-	5239														18%	-9.2	-9.5	-11.2
9-hydroxy-5,9-dimethyldec-4-enal	940-437-2	926-50-1	926501	-	-	5240														18%	-9.2	-9.5	-11.2
2,2-di(tetrahydrofuryl)propane	700-263-8	89686-69-1	89686691	-	-	5241														18%	-9.2	-9.6	-11.2
2-(acetylamino)-N-benzyl-3-methoxypropanamide	700-539-8	175481-26-2	175481262	-	-	5242														18%	-9.3	-9.6	-11.3
reaction products of 1,6-diisocyanatohexane with 2-[(2-metha	700-151-9	1101874-33-2	1101874332	-	-	5243														18%	-9.4	-9.7	-11.3
619-816-9	619-816-9	128446-33-3	128446333	-	-	5244														18%	-9.4	-9.7	-11.4
ethyl 2-allyl-2-cyano-3-methylhexanoate	700-062-5	33422-23-0	33422230	-	-	5245														18%	-9.4	-9.7	-11.4
2,7-naphthalenedisulfonic acid, 4-amino-5-hydroxy-, diazotizec	232-380-0	8011-86-7	8011867	-	-	5246														18%	-9.4	-9.7	-11.4
Reaction mass of benzyl 2-(2-methoxyethoxy)ethyl adipate and	940-202-4	1175612-76-6	1175612766	-	-	5247														18%	-9.5	-9.8	-11.5
Reaction products of 3-(trimethoxysilyl)propane-1-thiol and 5-i	700-534-0	117172-56-2	117172562	-	-	5248														18%	-9.5	-9.8	-11.5
[2,9,16,23-tetrachloro-29H,31H-phthalocyaninato(2-)-N29,N30	240-183-6	16040-69-0	16040690	-	-	5249														18%	-9.6	-9.9	-11.5
N-benzyl-2-bromo-3-methoxypropanamide	700-538-2	705283-58-5	705283585	-	-	5250														18%	-9.6	-9.9	-11.6
Alkanes, C10-13-iso-	271-366-9	68551-17-7	68551177	-	-	5251														18%	-9.6	-9.9	-11.6
tetrahydro-6-(3-pentenyl)-2H-pyran-2-one	251-201-7	32764-98-0	32764980	-	-	5252														18%	-9.7	-10.0	-11.6
5-cyclohexyl-2-methylpentan-1-ol	700-146-1	1141487-54-8	1141487548	-	-	5253														18%	-9.8	-10.1	-11.8
691-736-7	691-736-7	960495-42-5	960495425	-	-	5254														18%	-9.8	-10.1	-11.8
Reaction products of N-(1-oxododecyl)-L-glutamic acid and 2-o	700-285-8	1034015-52-5	1034015525	-	-	5255														18%	-9.9	-10.2	-11.8
Esterification products of N-Methyl-N-(1-oxotetradecyl)-β-alan	700-369-4	1085852-72-7	1085852727	-	-	5256														18%	-9.9	-10.2	-11.8
614-947-8	614-947-8	693217-63-9	693217639	-	-	5257														18%	-9.9	-10.2	-11.9
N,N-diisopropyl-3-(2-methoxy-5-methylphenyl)-3-phenylpropa	700-655-9	857288-56-3	857288563	-	-	5258														18%	-9.9	-10.2	-11.9
ethyl 3-amino-3-phenylpropanoate	613-206-6	6335-76-8	6335768	-	-	5259														18%	-10.1	-10.4	-12.0
Reaction products of chlorosulfonated reaction products of co	802-101-2	1246273-07-3	1246273073	-	-	5260														18%	-10.1	-10.4	-12.0
Reaction products of L-lysine and N-[(3S)-2,6-dioxotetrahydro-	688-011-2	1243654-79-6	1243654796	-	-	5261														18%	-10.1	-10.4	-12.0
6-[(2-{[5-({3-methyl-2,7-dioxo-1-[(3-sulfophenyl)carbonyl]-2,7-r	700-450-4	1007553-30-1	1007553301	-	-	5262														18%	-10.1	-10.4	-12.1
Reaction products of chlorosulfonated reaction products of co	700-449-9	1007578-75-7	1007578757	-	-	5263														18%	-10.1	-10.4	-12.1
N,N'-bis[2-hydroxy-3-(2,2,3,3-tetrafluoropropoxy)propyl]-N,N,N	700-737-4	1220100-43-5	1220100435	-	-	5264														18%	-10.1	-10.4	-12.1
700-904-1	700-904-1	1350725-68-6	1350725686	-	-	5265														18%	-10.1	-10.4	-12.1
2-{[2,2,4-trifluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}e	700-535-6	1190931-34-0	1190931340	-	-	5266														18%	-10.2	-10.5	-12.2
N-palmitoylisoleucine	627-025-5	101541-04-2	101541042	-	-	5267														18%	-10.5	-10.8	-12.5
3-(4-isobutylcyclohexyl)propanal	940-042-5	1254940-85-6	1254940856	-	-	5268														18%	-10.5	-10.8	-12.5
Pentadecanol, branched and linear	291-807-9	90480-71-0	90480710	-	-	5269														18%	-11.0	-11.3	-12.9
3-(hexyloxy)propane-1,2-diol	600-386-6	10305-38-1	10305381	-	-	5270														18%	-12.1	-12.4	-14.1
REACH - petroleum (not on SOLUTIONS' MLoS)																							
count							*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*326*	*280*	*326*	*326*	*326*	*326*	*326*
sum																	*1.9E+09*	*1.1E+09*	*6.0E+06*	*0%*			
standard deviation																					*1.4*	*1.4*	*1.4*
2.5-p																	*1.3E+02*	*6.7E+02*	*4.0E-01*	*0%*	*-11.6*	*-11.3*	*-13.7*
50-p																	*3.6E+05*	*3.9E+05*	*1.1E+03*	*0%*	*-8.2*	*-7.9*	*-10.3*
97.5-p																	*5.8E+07*	*2.6E+07*	*1.8E+05*	*0%*	*-6.0*	*-5.7*	*-8.1*
Fuels, diesel	269-822-7	68334-30-5	68334305	-	-	5272														0.3%	-5.2	-5.0	-7.3
Fuel oil, residual	270-675-6	68476-33-5	68476335	-	-	5273														0.3%	-5.5	-5.2	-7.6
Gasoline	289-220-8	86290-81-5	86290815	-	-	5274														0.3%	-5.5	-5.2	-7.7
Kerosine (petroleum)	232-366-4	8008-20-6	8008206	-	-	5275														0.3%	-5.8	-5.5	-7.9
Residues (petroleum), atmospheric	269-777-3	68333-22-2	68333222	-	-	5276														0.3%	-5.9	-5.6	-8.0
Residues (petroleum), atm. tower	265-045-2	64741-45-3	64741453	-	-	5277														0.3%	-5.9	-5.6	-8.0
Distillates (petroleum), full-range straight-run middle	272-341-5	68814-87-9	68814879	-	-	5278														0.3%	-6.0	-5.7	-8.1
Gas oils (petroleum), heavy vacuum	265-058-3	64741-57-7	64741577	-	-	5279														0.3%	-6.0	-5.7	-8.1
Naphtha (petroleum), full-range straight-run	265-042-6	64741-42-0	64741420	-	-	5280														0.3%	-6.0	-5.7	-8.1
Residues (petroleum), vacuum	265-057-8	64741-56-6	64741566	-	-	5281														0.3%	-6.0	-5.7	-8.1
Kerosine (petroleum), hydrodesulfurized	265-184-9	64742-81-0	64742810	-	-	5282														0.3%	-6.0	-5.7	-8.2
Distillates (petroleum), hydrodesulfurized middle	265-183-3	64742-80-9	64742809	-	-	5283														0.3%	-6.0	-5.7	-8.2
Distillates (petroleum), vacuum	274-685-1	70592-78-8	70592788	-	-	5284														0.3%	-6.3	-6.0	-8.4
Kerosine (petroleum), sweetened	294-799-5	91770-15-9	91770159	-	-	5285														0.3%	-6.3	-6.0	-8.4
Gas oils (petroleum), light vacuum	265-059-9	64741-58-8	64741588	-	-	5286														0.3%	-6.3	-6.0	-8.5
Naphtha (petroleum), catalytic reformed	273-271-8	68955-35-1	68955351	-	-	5287														0.3%	-6.4	-6.1	-8.5
Distillates (petroleum), petroleum residues vacuum	273-263-4	68955-27-1	68955271	-	-	5288														0.3%	-6.4	-6.1	-8.5
Gas oils (petroleum), straight-run	265-043-1	64741-43-1	64741431	-	-	5289														0.3%	-6.4	-6.1	-8.5
Asphalt	232-490-9	8052-42-4	8052424	-	-	5290														0.3%	-6.4	-6.1	-8.5
Distillates (petroleum), light catalytic cracked	265-060-4	64741-59-9	64741599	-	-	5291														0.3%	-6.4	-6.1	-8.5
Residues (petroleum), thermal cracked	265-081-9	64741-80-6	64741806	-	-	5292														0.3%	-6.4	-6.1	-8.5
Naphtha (petroleum), full-range reformed	272-895-8	68919-37-9	68919379	-	-	5293														0.3%	-6.5	-6.2	-8.6
Naphtha (petroleum), light catalytic cracked	265-056-2	64741-55-5	64741555	-	-	5294														0.3%	-6.5	-6.2	-8.6
Naphtha (petroleum), light straight-run	265-046-8	64741-46-4	64741464	-	-	5295														0.3%	-6.5	-6.2	-8.6
Naphtha (petroleum), hydrodesulfurized light	265-178-6	64742-73-0	64742730	-	-	5296														0.3%	-6.5	-6.2	-8.6
Fuels, diesel, no. 2	270-676-1	68476-34-6	68476346	-	-	5297														0.3%	-6.5	-6.2	-8.6
Naphtha (petroleum), heavy straight-run	265-041-0	64741-41-9	64741419	-	-	5298														0.3%	-6.5	-6.2	-8.7
Residues (petroleum), hydrocracked	265-076-1	64741-75-9	64741759	-	-	5299														0.3%	-6.6	-6.3	-8.7

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Lubricating oils	278-012-2	74869-22-0	74869220	-	-	5300														0.3%	-6.6	-6.3	-8.7
Gas oils (petroleum), hydrodesulfurized heavy vacuum	265-189-6	64742-86-5	64742865	-	-	5301														0.3%	-6.6	-6.3	-8.7
Naphtha (petroleum), hydrotreated heavy	265-150-3	64742-48-9	64742489	-	-	5302														0.3%	-6.6	-6.3	-8.7
Distillates (petroleum), hydrotreated middle	265-148-2	64742-46-7	64742467	-	-	5303														0.3%	-6.6	-6.3	-8.8
Gas oils (petroleum), hydrodesulfurized	265-182-8	64742-79-6	64742796	-	-	5304														0.3%	-6.7	-6.4	-8.8
Naphtha (petroleum), isomerization	265-073-5	64741-70-4	64741704	-	-	5305														0.3%	-6.7	-6.4	-8.8
Naphtha (petroleum), light catalytic cracked sweetened	295-441-0	92045-59-5	92045595	-	-	5306														0.3%	-6.8	-6.5	-8.9
Naphtha (petroleum), heavy catalytic cracked	265-055-7	64741-54-4	64741544	-	-	5307														0.3%	-6.8	-6.5	-8.9
Distillates (petroleum), light hydrocracked	265-078-2	64741-77-1	64741771	-	-	5308														0.3%	-6.8	-6.5	-8.9
Naphtha (petroleum), heavy catalytic reformed	265-070-9	64741-68-0	64741680	-	-	5309														0.3%	-6.8	-6.5	-8.9
Residues (petroleum), thermal cracked vacuum	295-518-9	92062-05-0	92062050	-	-	5310														0.3%	-6.8	-6.5	-9.0
Naphtha (petroleum), light catalytic reformed	265-065-1	64741-63-5	64741635	-	-	5311														0.3%	-6.8	-6.5	-9.0
Distillates (petroleum), heavy straight-run	272-817-2	68915-96-8	68915968	-	-	5312														0.3%	-6.9	-6.5	-9.0
Distillates (petroleum), straight-run middle	265-044-7	64741-44-2	64741442	-	-	5313														0.3%	-6.9	-6.6	-9.0
Distillates (petroleum), light thermal cracked	265-084-5	64741-82-8	64741828	-	-	5314														0.3%	-6.9	-6.6	-9.0
Naphtha (petroleum), hydrotreated light	265-151-9	64742-49-0	64742490	-	-	5315														0.3%	-6.9	-6.6	-9.0
Residues (petroleum), catalytic cracking	295-511-0	92061-97-7	92061977	-	-	5316														0.3%	-6.9	-6.6	-9.0
Naphtha (petroleum), unsweetened	272-186-3	68783-12-0	68783120	-	-	5317														0.3%	-6.9	-6.6	-9.0
Naphtha (petroleum), sweetened	265-089-2	64741-87-3	64741873	-	-	5318														0.3%	-6.9	-6.6	-9.1
Distillates (petroleum), heavy paraffinic	265-052-0	64741-51-1	64741511	-	-	5319														0.3%	-6.9	-6.6	-9.1
Fuel oil, no. 6	271-384-7	68553-00-4	68553004	-	-	5320														0.3%	-7.0	-6.6	-9.1
Naphtha (petroleum), full-range alkylate, butane-contg.	271-267-0	68527-27-5	68527275	-	-	5321														0.3%	-7.0	-6.7	-9.1
Naphtha (petroleum), hydrodesulfurized full-range	295-433-7	92045-52-8	92045528	-	-	5322														0.3%	-7.0	-6.7	-9.1
Distillates (petroleum), heavy hydrocracked	265-077-7	64741-76-0	64741760	-	-	5323														0.3%	-7.0	-6.7	-9.1
Asphalt, oxidized	265-196-4	64742-93-4	64742934	-	-	5324														0.3%	-7.0	-6.7	-9.1
Fuel oil, no. 2	270-671-4	68476-30-2	68476302	-	-	5325														0.3%	-7.0	-6.7	-9.1
Distillates (petroleum), hydrodesulfurized light catalytic cracke	269-781-5	68333-25-5	68333255	-	-	5326														0.3%	-7.0	-6.7	-9.2
Gas oils (petroleum), hydrotreated vacuum	265-162-9	64742-59-2	64742592	-	-	5327														0.3%	-7.1	-6.7	-9.2
Distillates (petroleum), light vacuum	274-684-6	70592-77-7	70592777	-	-	5328														0.3%	-7.1	-6.7	-9.2
Naphtha (petroleum), sweetened light	309-976-5	101795-01-1	101795011	-	-	5329														0.3%	-7.1	-6.8	-9.2
Distillates (petroleum), solvent-dewaxed heavy paraffinic	265-169-7	64742-65-0	64742650	-	-	5330														0.3%	-7.1	-6.8	-9.2
Naphtha (petroleum), hydrodesulfurized heavy	265-185-4	64742-82-1	64742821	-	-	5331														0.3%	-7.1	-6.8	-9.2
Residues (petroleum), vacuum, light	292-658-2	90669-76-4	90669764	-	-	5332														0.3%	-7.1	-6.8	-9.2
Hydrocarbons, C4, ethylene-manuf.-by-product	270-691-3	68476-52-8	68476528	-	-	5333														0.3%	-7.1	-6.8	-9.2
Fuel gases	270-667-2	68476-26-6	68476266	-	-	5334														0.3%	-7.1	-6.8	-9.2
xylene	215-535-7	1330-20-7	1330207	-	-	5335														0.3%	-7.1	-6.8	-9.3
Gasoline, pyrolysis, debutanizer bottoms	271-726-5	68606-10-0	68606100	-	-	5336														0.3%	-7.1	-6.8	-9.3
Distillates (petroleum), intermediate vacuum	274-683-0	70592-76-6	70592766	-	-	5337														0.3%	-7.1	-6.8	-9.3
Distillates (petroleum), heavy thermal cracked	265-082-4	64741-81-7	64741817	-	-	5338														0.3%	-7.1	-6.8	-9.3
Naphtha (petroleum), full-range alkylate	265-066-7	64741-64-6	64741646	-	-	5339														0.3%	-5.1	-5.4	-7.2
Naphtha (petroleum), light hydrocracked	265-071-4	64741-69-1	64741691	-	-	5340														0.3%	-7.2	-6.8	-9.3
Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-de	270-658-3	68475-70-7	68475707	-	-	5341														0.3%	-7.2	-6.9	-9.3
Naphtha (petroleum), heavy hydrocracked	265-079-8	64741-78-2	64741782	-	-	5342														0.3%	-7.2	-6.9	-9.3
Naphtha (petroleum), solvent-refined light	265-086-6	64741-84-0	64741840	-	-	5343														0.3%	-7.2	-6.9	-9.3
Residues (petroleum), topping plant, low-sulfur	271-763-7	68607-30-7	68607307	-	-	5344														0.3%	-7.2	-6.9	-9.3
Hydrocarbons, C4, steam-cracker distillate	295-405-4	92045-23-3	92045233	-	-	5345														0.3%	-7.2	-6.9	-9.3
Distillates (petroleum), solvent-refined heavy paraffinic	265-090-8	64741-88-4	64741884	-	-	5346														0.3%	-7.2	-6.9	-9.3
Aromatic hydrocarbons, C7-12, C8-rich	297-401-8	93571-75-6	93571756	-	-	5347														0.3%	-7.2	-6.9	-9.3
Naphtha (petroleum), light steam-cracked	265-187-5	64742-83-2	64742832	-	-	5348														0.3%	-7.2	-6.9	-9.3
Gas oils (petroleum), heavy atmospheric	272-184-2	68783-08-4	68783084	-	-	5349														0.3%	-7.3	-7.0	-9.4
Gases (petroleum), light steam-cracked, butadiene conc.	273-265-5	68955-28-2	68955282	-	-	5350														0.3%	-7.3	-7.0	-9.4
Distillates (petroleum), hydrotreated light	265-149-8	64742-47-8	64742478	-	-	5351														0.3%	-7.3	-7.0	-9.4
Naphtha (petroleum), light steam-cracked arom.	271-264-4	68527-23-1	68527231	-	-	5352														0.3%	-7.3	-7.0	-9.4
Clarified oils (petroleum), catalytic cracked	265-064-6	64741-62-4	64741624	-	-	5353														0.3%	-7.3	-7.0	-9.4
Distillates (petroleum), intermediate catalytic cracked	265-062-5	64741-60-2	64741602	-	-	5354														0.3%	-7.3	-7.0	-9.4
Gas oils (petroleum), thermal-cracked, hydrodesulfurized	295-411-7	92045-29-9	92045299	-	-	5355														0.3%	-7.3	-7.0	-9.5
Distillates (petroleum), hydrotreated heavy paraffinic	265-157-1	64742-54-7	64742547	-	-	5356														0.3%	-7.3	-7.0	-9.5
Gasoline, straight-run, topping-plant	271-727-0	68606-11-1	68606111	-	-	5357														0.3%	-7.3	-7.0	-9.5
Fuel oil, heavy, high-sulfur	295-396-7	92045-14-2	92045142	-	-	5358														0.3%	-7.4	-7.1	-9.5
Extracts (petroleum), heavy paraffinic distillate solvent	265-103-7	64742-04-7	64742047	-	-	5359														0.3%	-7.4	-7.1	-9.5
Hydrocarbons, ethylene-manuf.-by-product distn. residues	272-951-1	68921-67-5	68921675	-	-	5360														0.3%	-7.4	-7.1	-9.5
Hydrocarbons, C5-rich	270-695-5	68476-55-1	68476551	-	-	5361														0.3%	-7.4	-7.1	-9.5
Gasoline, C5-11, high-octane stabilized reformed	297-458-9	93572-29-3	93572293	-	-	5362														0.3%	-7.4	-7.1	-9.5
Distillates (petroleum), steam-cracked, C5-12 fraction	270-736-7	68477-53-2	68477532	-	-	5363														0.3%	-7.4	-7.1	-9.6
Gases (petroleum), crude distn. and catalytic cracking	273-563-5	68989-88-8	68989888	-	-	5364														0.3%	-7.5	-7.1	-9.6
Residues (petroleum), hydrodesulfurized atmospheric tower	265-181-2	64742-78-5	64742785	-	-	5365														0.3%	-7.5	-7.1	-9.6
Gas oils (petroleum), straight-run, high-boiling	272-818-8	68915-97-9	68915979	-	-	5366														0.3%	-7.5	-7.2	-9.6
Gas oils (petroleum), hydrodesulfurized light vacuum	265-190-1	64742-87-6	64742876	-	-	5367														0.3%	-7.5	-7.2	-9.6
Distillates (petroleum), light paraffinic	265-051-5	64741-50-0	64741500	-	-	5368														0.3%	-7.5	-7.2	-9.6
Naphtha	232-443-2	8030-30-6	8030306	-	-	5369														0.3%	-7.5	-7.2	-9.6
Residues (petroleum), heavy coker gas oil and vacuum gas oil	270-796-4	68478-17-1	68478171	-	-	5370														0.3%	-7.5	-7.2	-9.7
Residues (petroleum), steam-cracked	265-193-8	64742-90-1	64742901	-	-	5371														0.3%	-7.6	-7.2	-9.7
Gases (petroleum), refinery blend	272-183-7	68783-07-3	68783073	-	-	5372														0.3%	-7.6	-7.3	-9.7
Distillates (petroleum), light thermal cracked, debutanized aror	273-266-0	68955-29-3	68955293	-	-	5373														0.3%	-7.6	-7.3	-9.7
Distillates (petroleum), light straight-run gasoline fractionation	272-931-2	68921-08-4	68921084	-	-	5374														0.3%	-7.6	-7.3	-9.7

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Solvent naphtha (petroleum), light aliph.	265-192-2	64742-89-8	64742898	-	-	5375														0.3%	-7.6	-7.3	-9.7
Residual oils (petroleum), solvent deasphalted	265-096-0	64741-95-3	64741953	-	-	5376														0.3%	-7.6	-7.3	-9.7
Kerosine (petroleum), straight-run wide-cut	295-418-5	92045-37-9	92045379	-	-	5377														0.3%	-7.6	-7.3	-9.7
Hydrocarbons, C3	271-735-4	68606-26-8	68606268	-	-	5378														0.3%	-7.6	-7.3	-9.7
Hydrocarbons, C5-7, C6-rich, ethylene manuf. by-products	294-557-9	91723-50-1	91723501	-	-	5379														0.3%	-7.6	-7.3	-9.7
Naphtha (petroleum), full-range coker	270-991-4	68513-02-0	68513020	-	-	5380														0.3%	-7.7	-7.4	-9.8
Distillates (petroleum), naphtha steam cracking-derived, hydro	295-311-3	91995-50-5	91995505	-	-	5381														0.3%	-7.7	-7.4	-9.8
Naphtha (petroleum), steam-cracked middle arom.	271-138-9	68516-20-1	68516201	-	-	5382														0.3%	-7.7	-7.4	-9.8
Natural gas condensates (petroleum)	265-047-3	64741-47-5	64741475	-	-	5383														0.3%	-7.7	-7.4	-9.8
Hydrocarbons, C"e5, C5-6-rich	270-690-8	68476-50-6	68476506	-	-	5384														0.3%	-7.7	-7.4	-9.8
Distillates (petroleum), heavy catalytic cracked	265-063-0	64741-61-3	64741613	-	-	5385														0.3%	-7.7	-7.4	-9.8
Gasoline, pyrolysis, hydrogenated	302-639-3	94114-03-1	94114031	-	-	5386														0.3%	-7.7	-7.4	-9.8
Slack wax (petroleum)	265-165-5	64742-61-6	64742616	-	-	5387														0.3%	-7.7	-7.4	-9.8
Fuel oil, residues-straight-run gas oils, high-sulfur	270-674-0	68476-32-4	68476324	-	-	5388														0.3%	-7.8	-7.4	-9.9
Distillates (petroleum), solvent-refined light paraffinic	265-091-3	64741-89-5	64741895	-	-	5389														0.3%	-7.8	-7.5	-9.9
Petroleum products, hydrofiner-powerformer reformates	271-058-4	68514-79-4	68514794	-	-	5390														0.3%	-7.8	-7.5	-9.9
Solvent naphtha (petroleum), light arom.	265-199-0	64742-95-6	64742956	-	-	5391														0.3%	-7.8	-7.5	-9.9
Gasoline, natural	232-349-1	8006-61-9	8006619	-	-	5392														0.3%	-7.8	-7.5	-9.9
Hydrocarbons, C3-11, catalytic cracker distillates	270-686-6	68476-46-0	68476460	-	-	5393														0.3%	-7.8	-7.5	-9.9
Residual oils (petroleum), solvent-refined	265-101-6	64742-01-4	64742014	-	-	5394														0.3%	-7.8	-7.5	-9.9
Residues (petroleum), steam-cracked light	271-013-9	68513-69-9	68513699	-	-	5395														0.3%	-7.8	-7.5	-9.9
Fuel gases, refinery	269-640-8	68308-27-0	68308270	-	-	5396														0.3%	-7.8	-7.5	-9.9
Distillates (petroleum), C6-rich	296-903-4	93165-19-6	93165196	-	-	5397														0.3%	-7.8	-7.5	-9.9
Naphtha (petroleum), light, sweetened	272-206-0	68783-66-4	68783664	-	-	5398														0.3%	-7.8	-7.5	-9.9
Residual oils (petroleum), solvent-dewaxed	265-166-0	64742-62-7	64742627	-	-	5399														0.3%	-7.8	-7.5	-10.0
Petroleum gases, liquefied	270-704-2	68476-85-7	68476857	-	-	5400														0.3%	-7.8	-7.5	-10.0
Naphtha (petroleum), light thermal cracked	265-075-6	64741-74-8	64741748	-	-	5401														0.3%	-7.8	-7.5	-10.0
Fuel oil, no. 4	270-673-5	68476-31-3	68476313	-	-	5402														0.3%	-7.9	-7.6	-10.0
Gases (petroleum), depropanizer dry, propene-rich	270-772-3	68477-90-7	68477907	-	-	5403														0.3%	-7.9	-7.6	-10.0
Hydrocarbons, C4-6, depentanizer lights, arom. hydrotreater	295-298-4	91995-38-9	91995389	-	-	5404														0.3%	-7.9	-7.6	-10.0
Residues (petroleum), vacuum distn. residue hydrogenation	309-713-4	100684-40-0	100684400	-	-	5405														0.3%	-7.9	-7.6	-10.0
Aromatic hydrocarbons, C8, catalytic reforming-derived	295-279-0	91995-18-5	91995185	-	-	5406														0.3%	-7.9	-7.6	-10.0
Condensates (petroleum), vacuum tower	265-049-4	64741-49-7	64741497	-	-	5407														0.3%	-7.9	-7.6	-10.0
Naphtha (petroleum), heavy thermal cracked	265-085-0	64741-83-9	64741839	-	-	5408														0.3%	-7.9	-7.6	-10.0
Distillates (petroleum), hydrotreated light paraffinic	265-158-7	64742-55-8	64742558	-	-	5409														0.3%	-7.9	-7.6	-10.0
Distillates (petroleum), hydrodesulfurized middle coker	309-865-1	101316-59-0	101316590	-	-	5410														0.3%	-7.9	-7.6	-10.0
Paraffin waxes and Hydrocarbon waxes	232-315-6	8002-74-2	8002742	-	-	5411														0.3%	-7.9	-7.6	-10.0
Distillates (petroleum), steam-cracked, C8-12 fraction	270-737-2	68477-54-3	68477543	-	-	5412														0.3%	-7.9	-7.6	-10.0
Residues (petroleum), hydrodesulfurized vacuum	265-188-0	64742-85-4	64742854	-	-	5413														0.3%	-7.9	-7.6	-10.0
Aromatic hydrocarbons, C7-8, ethylene-manuf.-by-product	292-699-6	90989-43-8	90989438	-	-	5414														0.3%	-8.0	-7.6	-10.1
Hydrocarbons, C4, 1,3-butadiene- and isobutene-free	306-004-1	95465-89-7	95465897	-	-	5415														0.3%	-8.0	-7.6	-10.1
Lubricating oils (petroleum), C20-50, hydrotreated neutral oil-b	276-738-4	72623-87-1	72623871	-	-	5416														0.3%	-8.0	-7.7	-10.1
Solvent naphtha (petroleum), hydrocracked heavy arom.	309-881-9	101316-80-7	101316807	-	-	5417														0.3%	-8.0	-7.7	-10.1
Residues (petroleum), distn. residue hydrogenation	309-712-9	100684-39-7	100684397	-	-	5418														0.3%	-8.0	-7.7	-10.1
Solvent naphtha (petroleum), heavy arom.	265-198-5	64742-94-5	64742945	-	-	5419														0.3%	-8.0	-7.7	-10.1
Extracts (petroleum), catalytic reformed light naphtha solvent	295-331-2	91995-68-5	91995685	-	-	5420														0.3%	-8.0	-7.7	-10.1
Lubricating oils (petroleum), C24-50, solvent-extd., dewaxed, h	309-877-7	101316-72-7	101316727	-	-	5421														0.3%	-8.0	-7.7	-10.1
Distillates (petroleum), hydrotreated middle, intermediate boili	270-092-7	68410-96-8	68410968	-	-	5422														0.3%	-8.0	-7.7	-10.1
Distillates (petroleum), hydrotreated heavy naphthenic	265-155-0	64742-52-5	64742525	-	-	5423														0.3%	-8.0	-7.7	-10.2
Residues (petroleum), steam-cracked light, arom.	310-057-6	102110-55-4	102110554	-	-	5424														0.3%	-8.0	-7.7	-10.2
Naphtha (petroleum), light, C5-rich, sweetened	295-442-6	92045-60-8	92045608	-	-	5425														0.3%	-8.1	-7.8	-10.2
Gases (petroleum), catalytic cracked overheads	270-071-2	68409-99-4	68409994	-	-	5426														0.3%	-8.1	-7.8	-10.2
White mineral oil (petroleum)	232-455-8	8042-47-5	8042475	-	-	5427														0.3%	-8.1	-7.8	-10.2
Hydrocarbons, C3-4-rich, petroleum distillate	270-990-9	68512-91-4	68512914	-	-	5428														0.3%	-8.1	-7.8	-10.2
Slack wax (petroleum), clay-treated	292-660-3	90669-78-6	90669786	-	-	5429														0.3%	-8.1	-7.8	-10.2
Distillates (petroleum), hydrotreated light naphthenic	265-156-6	64742-53-6	64742536	-	-	5430														0.3%	-8.1	-7.8	-10.2
Naphtha (petroleum), heavy catalytic cracked, sweetened	295-431-6	92045-50-6	92045506	-	-	5431														0.3%	-8.1	-7.8	-10.2
Aromatic hydrocarbons, C8	292-694-9	90989-38-1	90989381	-	-	5432														0.3%	-8.1	-7.8	-10.3
Gases (petroleum), C3-5 olefinic-paraffinic alkylation feed	270-765-5	68477-83-8	68477838	-	-	5433														0.3%	-8.1	-7.8	-10.3
Hydrocarbons, C7-12, C>9-arom.-rich, reforming heavy fraction	297-465-7	93572-35-1	93572351	-	-	5434														0.3%	-8.2	-7.9	-10.3
Extracts (petroleum), residual oil solvent	265-110-5	64742-10-5	64742105	-	-	5435														0.3%	-8.2	-7.9	-10.3
Naphtha (petroleum), hydrodesulfurized full-range coker	309-879-8	101316-76-1	101316761	-	-	5436														0.3%	-8.2	-7.9	-10.3
Distillates (petroleum), solvent-dewaxed light paraffinic	265-159-2	64742-56-9	64742569	-	-	5437														0.3%	-8.2	-7.9	-10.3
Paraffin waxes (petroleum), hydrotreated	265-154-5	64742-51-4	64742514	-	-	5438														0.3%	-8.2	-7.9	-10.3
613-683-0	613-683-0	64741-72-6	64741726	-	-	5439														0.3%	-8.2	-7.9	-10.3
Naphtha (petroleum), catalytic reformed light, arom.-free fract	285-510-3	85116-59-2	85116592	-	-	5440														0.3%	-8.2	-7.9	-10.3
Hydrocarbons, C6-rich, hydrotreated light naphtha distillates, s	309-871-4	101316-67-0	101316670	-	-	5441														0.3%	-8.2	-7.9	-10.3
Extracts (petroleum), light paraffinic distillate solvent	265-104-2	64742-05-8	64742058	-	-	5442														0.3%	-8.2	-7.9	-10.3
Gases (petroleum), C3-4	268-629-5	68131-75-9	68131759	-	-	5443														0.3%	-8.2	-7.9	-10.3
Hydrocarbons, C5-11, nonaroms.-rich, reforming light fraction	297-466-2	93572-36-2	93572362	-	-	5444														0.3%	-8.2	-7.9	-10.3
Distillates (petroleum), straight-run light	270-077-5	68410-05-9	68410059	-	-	5445														0.3%	-8.2	-7.9	-10.3
Hydrocarbons, C6-7, naphtha-cracking, solvent-refined	295-446-8	92045-64-2	92045642	-	-	5446														0.3%	-8.2	-7.9	-10.4
Distillates (petroleum), hydrotreated light catalytic cracked	272-930-7	68921-07-3	68921073	-	-	5447														0.3%	-8.3	-7.9	-10.4
Fuel gases, crude oil distillates	270-670-9	68476-29-9	68476299	-	-	5448														0.3%	-8.3	-7.9	-10.4
Naphtha (petroleum), isomerization, C6-fraction	295-440-5	92045-58-4	92045584	-	-	5449														0.3%	-8.3	-7.9	-10.4

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Residues (petroleum), light vacuum	270-984-6	68512-62-9	68512629	-	-	5450														0.3%	-8.3	-8.0	-10.4
Naphtha (petroleum), light catalytic reformed, arom.-free	270-993-5	68513-03-1	68513031	-	-	5451														0.3%	-8.3	-8.0	-10.4
Naphtha (petroleum), steam-cracked, hydrotreated, C9-10-aro	292-637-8	90641-13-7	90641137	-	-	5452														0.3%	-8.3	-8.0	-10.4
Distillates (petroleum), sweetened middle	265-088-7	64741-86-2	64741862	-	-	5453														0.3%	-8.3	-8.0	-10.4
Distillates (petroleum), cracked steam-cracked petroleum distil	270-727-8	68477-38-3	68477383	-	-	5454														0.3%	-8.3	-8.0	-10.4
Aromatic hydrocarbons, distn. residues, naphthalene-rich	308-487-4	98072-36-7	98072367	-	-	5455														0.3%	-8.3	-8.0	-10.4
Distillates (petroleum), catalytic reformed depentanizer	270-660-4	68475-79-6	68475796	-	-	5456														0.3%	-8.3	-8.0	-10.4
Naphtha (petroleum), light alkylate	265-068-8	64741-66-8	64741668	-	-	5457														0.3%	-8.3	-8.0	-10.4
Distillates (petroleum), cracked stripped steam-cracked petrole	270-728-3	68477-39-4	68477394	-	-	5458														0.3%	-8.3	-8.0	-10.4
Residual oils (petroleum), hydrotreated	265-160-8	64742-57-0	64742570	-	-	5459														0.3%	-8.3	-8.0	-10.4
Residual oils (petroleum)	298-754-0	93821-66-0	93821660	-	-	5460														0.3%	-8.3	-8.0	-10.5
Distillates (petroleum), light steam-cracked naphtha	270-662-5	68475-80-9	68475809	-	-	5461														0.3%	-8.3	-8.0	-10.5
gases (petroleum), C3-4, isobutane-rich	270-724-1	68477-33-8	68477338	-	-	5462														0.3%	-8.3	-8.0	-10.5
Foots oil (petroleum)	265-171-8	64742-67-2	64742672	-	-	5463														0.3%	-8.4	-8.1	-10.5
Naphtha (petroleum), hydrotreated light steam-cracked	295-438-4	92045-57-3	92045573	-	-	5464														0.3%	-8.4	-8.1	-10.5
Hydrocarbons, C4-11, naphtha-cracking, arom.-free	295-445-2	92045-63-1	92045631	-	-	5465														0.3%	-8.4	-8.1	-10.5
Distillates (petroleum), light naphthenic	265-053-6	64741-52-2	64741522	-	-	5466														0.3%	-8.4	-8.1	-10.5
Paraffin oils (petroleum), catalytic dewaxed heavy	265-174-4	64742-70-7	64742707	-	-	5467														0.3%	-8.4	-8.1	-10.6
Distillates (petroleum), heavy naphthenic	265-054-1	64741-53-3	64741533	-	-	5468														0.3%	-8.5	-8.2	-10.6
Petrolatum	232-373-2	8009-03-8	8009038	-	-	5469														0.3%	-8.5	-8.2	-10.6
Slack wax (petroleum), hydrotreated	295-523-6	92062-09-4	92062094	-	-	5470														0.3%	-8.5	-8.2	-10.6
Alkanes, C12-26-branched and linear	292-454-3	90622-53-0	90622530	-	-	5471														0.3%	-8.5	-8.2	-10.6
Extracts (petroleum), solvent-refined heavy paraffinic distillate	272-180-0	68783-04-0	68783040	-	-	5472														0.3%	-8.5	-8.2	-10.6
Hydrocarbons, C5-unsatd.	273-308-8	68956-55-8	68956558	-	-	5473														0.3%	-8.5	-8.2	-10.6
Hydrocarbons, C4-12, naphtha-cracking, hydrotreated	295-443-1	92045-61-9	92045619	-	-	5474														0.3%	-8.5	-8.2	-10.7
Gases (petroleum), C2-4, sweetened	272-205-5	68783-65-3	68783653	-	-	5475														0.3%	-8.5	-8.2	-10.7
Hydrocarbons, steam-cracking tar middle	289-222-9	86290-83-7	86290837	-	-	5476														0.3%	-8.6	-8.3	-10.7
Naphtha (petroleum), arom	271-635-0	68603-08-7	68603087	-	-	5477														0.3%	-8.6	-8.3	-10.7
Paraffin waxes and Hydrocarbon waxes, microcryst.	264-038-1	63231-60-7	63231607	-	-	5478														0.3%	-8.7	-8.4	-10.8
614-725-0	614-725-0	68783-11-9	68783119	-	-	5479														0.3%	-8.7	-8.4	-10.8
Gas oils (petroleum), steam-cracked	271-260-2	68527-18-4	68527184	-	-	5480														0.3%	-8.7	-8.4	-10.8
Naphtha (petroleum), catalytic dewaxed	265-170-2	64742-66-1	64742661	-	-	5481														0.3%	-8.7	-8.4	-10.8
Alkenes, C8-10-branched, C9-rich	307-301-9	97593-01-6	97593016	-	-	5482														0.3%	-8.7	-8.4	-10.8
Lubricating oils, used, vacuum distd.	295-422-7	92045-41-5	92045415	-	-	5483														0.3%	-8.8	-8.5	-10.9
Alkenes, C10-14-branched and linear, C12-rich	298-697-1	93821-12-6	93821126	-	-	5484														0.3%	-8.8	-8.5	-10.9
Hydrocarbons, C2-4, C3-rich	270-689-2	68476-49-3	68476493	-	-	5485														0.3%	-8.8	-8.5	-10.9
Distillates (petroleum), cracked, ethylene manuf. by-product, C	305-586-4	94733-07-0	94733070	-	-	5486														0.3%	-8.8	-8.5	-10.9
Paraffin waxes (petroleum), clay-treated	265-145-6	64742-43-4	64742434	-	-	5487														0.3%	-8.8	-8.5	-10.9
Raffinates (petroleum), catalytic reformer ethylene glycol-wate	270-088-5	68410-71-9	68410719	-	-	5488														0.3%	-8.8	-8.5	-10.9
Hydrocarbons, C4, n-butene conc.	306-005-7	95465-90-0	95465900	-	-	5489														0.3%	-8.8	-8.5	-11.0
Hydrocarbons, C3-6, C5-rich, steam-cracked naphtha	310-012-0	102110-14-5	102110145	-	-	5490														0.3%	-8.9	-8.5	-11.0
Gases (petroleum), catalytic-cracked gas oil depropanizer bottc	270-752-4	68477-71-4	68477714	-	-	5491														0.3%	-8.9	-8.6	-11.0
Petrolatum (petroleum), hydrotreated	295-459-9	92045-77-7	92045777	-	-	5492														0.3%	-8.9	-8.6	-11.0
Residues (petroleum), catalytic reformer fractionator	265-069-3	64741-67-9	64741679	-	-	5493														0.3%	-8.9	-8.6	-11.0
Lubricating oils (petroleum), C15-30, hydrotreated neutral oil-b	276-737-9	72623-86-0	72623860	-	-	5494														0.3%	-8.9	-8.6	-11.0
Alkenes, C9-11, C10-rich	271-213-6	68526-56-7	68526567	-	-	5495														0.3%	-8.9	-8.6	-11.0
Gases (petroleum), refinery	272-338-9	68814-67-5	68814675	-	-	5496														0.3%	-8.9	-8.6	-11.0
Extracts (petroleum), deasphalted vacuum residue solvent	295-332-8	91995-70-9	91995709	-	-	5497														0.3%	-8.9	-8.6	-11.0
Lubricating oils (petroleum), C>25, solvent-extd., deasphalted,	309-874-0	101316-69-2	101316692	-	-	5498														0.3%	-9.0	-8.7	-11.1
Gases (petroleum), deisobutanizer tower overheads	270-769-7	68477-87-2	68477872	-	-	5499														0.3%	-9.0	-8.7	-11.1
Dec-1-ene, trimers, hydrogenated	500-393-3	157707-86-3	157707863	-	-	5500														0.3%	-9.0	-8.7	-11.2
Hydrocarbons, C6-8, hydrogenated sorption-dearomatized, tol	309-870-9	101316-66-9	101316669	-	-	5501														0.3%	-9.1	-8.8	-11.2
Extracts (petroleum), light naphtha solvent	265-100-0	64741-99-7	64741997	-	-	5502														0.3%	-9.1	-8.8	-11.2
Solvent naphtha (petroleum), heavy aliph.	265-200-4	64742-96-7	64742967	-	-	5503														0.3%	-9.1	-8.8	-11.2
Extracts (petroleum), heavy naphtha solvent	265-099-7	64741-98-6	64741986	-	-	5504														0.3%	-9.1	-8.8	-11.3
Distillates (petroleum), cracked stripped steam-cracked petrole	270-729-9	68477-40-7	68477407	-	-	5505														0.3%	-9.1	-8.8	-11.3
Alkenes, C8-10, C9-rich	271-212-0	68526-55-6	68526556	-	-	5506														0.3%	-9.2	-8.9	-11.3
dodecene	246-922-9	25378-22-7	25378227	-	-	5507														0.3%	-9.2	-8.9	-11.3
Alkenes, C10-14	288-213-7	85681-75-0	85681750	-	-	5508														0.3%	-9.2	-8.9	-11.3
Distillates (petroleum), heat-soaked steam-cracked naphtha, C!	295-302-4	91995-41-4	91995414	-	-	5509														0.3%	-9.2	-8.9	-11.3
Hydrocarbon waxes (petroleum), hydrotreated microcryst.	265-163-4	64742-60-5	64742605	-	-	5510														0.3%	-9.2	-8.9	-11.3
Hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene	293-263-8	91053-01-9	91053019	-	-	5511														0.3%	-9.3	-9.0	-11.4
Hydrocarbon waxes (petroleum), clay-treated microcryst.	265-144-0	64742-42-3	64742423	-	-	5512														0.3%	-9.3	-9.0	-11.5
Distillates (petroleum), polymd. steam-cracked petroleum distil	270-735-1	68477-50-9	68477509	-	-	5513														0.3%	-9.3	-9.0	-11.5
Paraffin oils (petroleum), catalytic dewaxed light	265-176-5	64742-71-8	64742718	-	-	5514														0.3%	-9.4	-9.0	-11.5
Alkanes, C14-17	292-449-6	90622-47-2	90622472	-	-	5515														0.3%	-9.4	-9.1	-11.5
Hydrocarbons, C4, 1,3-butadiene-free, polymd., dibutylene frac	293-261-7	91052-99-2	91052992	-	-	5516														0.3%	-9.4	-9.1	-11.5
Gases (petroleum), butane splitter overheads	270-750-3	68477-69-0	68477690	-	-	5517														0.3%	-9.4	-9.1	-11.5
Distillates (petroleum), solvent-refined heavy naphthenic	265-097-6	64741-96-4	64741964	-	-	5518														0.3%	-9.4	-9.1	-11.5
Hydrocarbons, C4, butane conc., n-butene-contg.	306-006-2	95465-91-1	95465911	-	-	5519														0.3%	-9.4	-9.1	-11.5
Lubricating oils (petroleum), C18-40, solvent-dewaxed hydrocra	305-594-8	94733-15-0	94733150	-	-	5520														0.3%	-9.4	-9.1	-11.5
Natural gas (petroleum), raw liq. mix	265-048-9	64741-48-6	64741486	-	-	5521														0.3%	-9.4	-9.1	-11.5
Hydrocarbons, C4-6, C5-rich	270-684-5	68476-43-7	68476437	-	-	5522														0.3%	-9.4	-9.1	-11.5
Distillates (petroleum), hydrodesulfurized thermal cracked mid	285-505-6	85116-53-6	85116536	-	-	5523														0.3%	-9.5	-9.1	-11.6
tridecene	246-919-2	25377-82-6	25377826	-	-	5524														0.3%	-9.5	-9.2	-11.6

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Distillates (petroleum), catalytic reformed hydrotreated light, C	285-509-8	85116-58-1	85116581	-	-	5525														0.3%	-9.5	-9.2	-11.6
Gases (petroleum), straight-run stabilizer off	272-883-2	68919-10-8	68919108	-	-	5526														0.3%	-9.5	-9.2	-11.6
Solvent naphtha (petroleum), medium aliph.	265-191-7	64742-88-7	64742887	-	-	5527														0.3%	-9.5	-9.2	-11.6
tetradecene	248-130-9	26952-13-6	26952136	-	-	5528														0.3%	-9.6	-9.2	-11.7
Gas oils (petroleum), hydrotreated light vacuum	295-407-5	92045-24-4	92045244	-	-	5529														0.3%	-9.6	-9.3	-11.7
Hydrocarbons, C9-14, ethylene-manuf.-by-product	271-035-9	68514-34-1	68514341	-	-	5530														0.3%	-9.6	-9.3	-11.7
Hydrocarbons, C9-16, hydrotreated, dearomatized	297-854-1	93763-35-0	93763350	-	-	5531														0.3%	-9.6	-9.3	-11.7
Residues (petroleum), alkylation splitter, C4-rich	271-010-2	68513-66-6	68513666	-	-	5532														0.3%	-9.6	-9.3	-11.7
Paraffin waxes and Hydrocarbon waxes, microcryst., hydrotrea	295-458-3	92045-76-6	92045766	-	-	5533														0.3%	-9.7	-9.4	-11.8
Naphtha (petroleum), light steam-cracked, debenzenized, C8-1	270-790-1	68478-10-4	68478104	-	-	5534														0.3%	-9.7	-9.4	-11.8
Petroleum gases, liquefied, sweetened, C4 fraction	295-463-0	92045-80-2	92045802	-	-	5535														0.3%	-9.7	-9.4	-11.8
Hydrocarbons, C17-30, hydrotreated distillates, distn. lights	308-132-3	97862-82-3	97862823	-	-	5536														0.3%	-9.7	-9.4	-11.8
Foots oil (petroleum), hydrotreated	295-394-6	92045-12-0	92045120	-	-	5537														0.3%	-9.7	-9.4	-11.9
Gas oils, paraffinic	300-227-8	93924-33-5	93924335	-	-	5538														0.3%	-9.7	-9.4	-11.9
Gases (petroleum), catalytic reformed naphtha stripper overhe	270-759-2	68477-77-0	68477770	-	-	5539														0.3%	-9.8	-9.5	-11.9
Benzenesulfonic acid, C16-24-alkyl derivs.	274-262-1	70024-67-8	70024678	-	-	5540														0.3%	-9.8	-9.5	-11.9
isoheptane	250-610-8	31394-54-4	31394544	-	-	5541														0.3%	-9.9	-9.6	-12.0
Sulfonic acids, petroleum, sodium salts	271-781-5	68608-26-4	68608264	-	-	5542														0.3%	-9.9	-9.6	-12.0
Naphtha (petroleum), hydrodesulfurized light, dearomatized	295-434-2	92045-53-9	92045539	-	-	5543														0.3%	-9.9	-9.6	-12.0
Distillates (petroleum), dewaxed light paraffinic, hydrotreated	295-301-9	91995-40-3	91995403	-	-	5544														0.3%	-9.9	-9.6	-12.0
Hydrocarbons, C4, 1,3-butadiene-free, polymd., dibutylene frac	297-626-1	93685-78-0	93685780	-	-	5545														0.3%	-10.0	-9.6	-12.1
Benzenesulfonic acid, mono-C16-24-alkyl derivs., calcium salts	274-263-7	70024-69-0	70024690	-	-	5546														0.3%	-10.0	-9.7	-12.1
Paraffins (petroleum), normal C>10	265-232-9	64771-71-7	64771717	-	-	5547														0.3%	-10.0	-9.7	-12.1
Benzenesulfonic acid, C14-44-branched and linear alkyl derivs.,	294-233-7	91696-74-1	91696741	-	-	5548														0.3%	-10.0	-9.7	-12.1
Hydrocarbons, C6-11, hydrotreated, dearomatized	297-852-0	93763-33-8	93763338	-	-	5549														0.3%	-10.0	-9.7	-12.1
Gases (petroleum), C1-5, wet	271-624-0	68602-83-5	68602835	-	-	5550														0.3%	-10.1	-9.7	-12.2
604-769-9	604-769-9	151006-63-2	151006632	-	-	5551														0.3%	-10.1	-9.8	-12.2
Naphthenic acids	215-662-8	1338-24-5	1338245	-	-	5552														0.3%	-10.1	-9.8	-12.2
618-143-8	618-143-8	883233-93-0	883233930	-	-	5553														0.3%	-10.1	-9.8	-12.2
Alkenes, C15-18	297-797-2	93762-80-2	93762802	-	-	5554														0.3%	-10.2	-9.9	-12.3
Distillates (petroleum), solvent-refined light naphthenic	265-098-1	64741-97-5	64741975	-	-	5555														0.3%	-10.2	-9.9	-12.4
618-141-7	618-141-7	883233-48-5	883233485	-	-	5556														0.3%	-10.3	-9.9	-12.4
Hydrocarbons, C4, 1,3-butadiene-free, polymd., tetraisobutyler	293-262-2	91053-00-8	91053008	-	-	5557														0.3%	-10.3	-9.9	-12.4
Petrolatum (petroleum), oxidized	265-206-7	64743-01-7	64743017	-	-	5558														0.3%	-10.3	-10.0	-12.4
Sulfonic acids, petroleum, calcium salts	263-093-9	61789-86-4	61789864	-	-	5559														0.3%	-10.3	-10.0	-12.4
Lubricating oils (petroleum), base oils, paraffinic	297-474-6	93572-43-1	93572431	-	-	5560														0.3%	-10.3	-10.0	-12.4
Benzenesulfonic acid, C10-16-alkyl derivs., calcium salts	271-529-4	68584-23-6	68584236	-	-	5561														0.3%	-10.3	-10.0	-12.4
Distillates (petroleum), chemically neutralized light	265-132-5	64742-31-0	64742310	-	-	5562														0.3%	-10.3	-10.0	-12.4
Benzene, ethylenated, residues	273-494-0	68987-42-8	68987428	-	-	5563														0.3%	-10.3	-10.0	-12.5
Lubricating oils (petroleum), C20-50, hydrotreated neutral oil-b	276-736-3	72623-85-9	72623859	-	-	5564														0.3%	-10.4	-10.1	-12.5
Ligroine	232-453-7	8032-32-4	8032324	-	-	5565														0.3%	-10.4	-10.1	-12.5
Paraffin oils	232-384-2	8012-95-1	8012951	-	-	5566														0.3%	-10.4	-10.1	-12.5
618-142-2	618-142-2	883233-91-8	883233918	-	-	5567														0.3%	-10.4	-10.1	-12.5
Residues, steam cracked, thermally treated	308-733-0	98219-64-8	98219648	-	-	5568														0.3%	-10.4	-10.1	-12.5
tetrapropylenebenzene	246-772-4	25265-78-5	25265785	-	-	5569														0.3%	-10.5	-10.2	-12.6
Distillates (petroleum), solvent-refined hydrotreated heavy, hy	305-588-5	94733-08-1	94733081	-	-	5570														0.3%	-10.5	-10.2	-12.6
Benzenesulfonic acid, C10-60-alkyl derivs., calcium salts	290-636-7	90194-27-7	90194277	-	-	5571														0.3%	-10.5	-10.2	-12.6
Benzenesulfonic acid, C10-16-alkyl derivs.	271-528-9	68584-22-5	68584225	-	-	5572														0.3%	-10.5	-10.2	-12.6
octene	246-920-8	25377-83-7	25377837	-	-	5573														0.3%	-10.7	-10.4	-12.8
Hydrocarbon waxes (petroleum), oxidized	265-205-1	64743-00-6	64743006	-	-	5574														0.3%	-10.7	-10.4	-12.8
Residual oils (petroleum), catalytic dewaxed	294-843-3	91770-57-9	91770579	-	-	5575														0.3%	-10.7	-10.4	-12.8
Paraffins (petroleum), normal C5-20	265-233-4	64771-72-8	64771728	-	-	5576														0.3%	-10.7	-10.4	-12.8
Foots oil (petroleum), clay-treated	300-226-2	93924-32-4	93924324	-	-	5577														0.3%	-10.8	-10.4	-12.9
Sulfonic acids, petroleum, magnesium salts	263-094-4	61789-87-5	61789875	-	-	5578														0.3%	-10.8	-10.5	-12.9
Benzenesulfonic acid, C10-16-alkyl derivs., magnesium salts	271-533-6	68584-26-9	68584269	-	-	5579														0.3%	-10.8	-10.5	-12.9
Residual oils (petroleum), hydrotreated solvent dewaxed	292-656-1	90669-74-2	90669742	-	-	5580														0.3%	-10.8	-10.5	-12.9
Sulfonic acids, petroleum	263-092-3	61789-85-3	61789853	-	-	5581														0.3%	-10.8	-10.5	-13.0
Distillates (petroleum), clay-treated heavy naphthenic	265-146-1	64742-44-5	64742445	-	-	5582														0.3%	-10.8	-10.5	-13.0
Naphtha (petroleum), heavy alkylate	265-067-2	64741-65-7	64741657	-	-	5583														0.3%	-10.9	-10.6	-13.1
Lubricating oils, used, distd.	295-421-1	92045-40-4	92045404	-	-	5584														0.3%	-11.0	-10.7	-13.1
2-Methylpropene, trimers	500-001-0	7756-94-7	7756947	-	-	5585														0.3%	-11.0	-10.7	-13.1
Petrolatum (petroleum), clay-treated	309-706-6	100684-33-1	100684331	-	-	5586														0.3%	-11.1	-10.8	-13.2
Petrolatum (petroleum), oxidized, Bu ester	292-642-5	90669-48-0	90669480	-	-	5587														0.3%	-11.5	-11.2	-13.6
Hydrocarbon waxes (petroleum), oxidized, Me esters, calcium s	271-638-7	68603-11-2	68603112	-	-	5588														0.3%	-11.6	-11.3	-13.7
Sulfonic acids, petroleum, barium salts	263-140-3	61790-48-5	61790485	-	-	5589														0.3%	-11.6	-11.3	-13.7
Benzenesulfonic acid, di-C10-18-alkyl derivs., barium salts	298-635-3	93820-55-4	93820554	-	-	5590														0.3%	-11.6	-11.3	-13.7
800-484-0	800-484-0	154518-38-4	154518384	-	-	5591														0.3%	-11.6	-11.3	-13.8
Hydrocarbons, C4, 1,3-butadiene-free, polymd., pentaisobutyle	297-627-7	93685-79-1	93685791	-	-	5592														0.3%	-11.7	-11.4	-13.8
Alkenes, C14-15	297-796-7	93762-79-9	93762799	-	-	5593														0.3%	-11.7	-11.4	-13.8
Extracts (petroleum), heavy paraffinic distillates, solvent-deasp	272-342-0	68814-89-1	68814891	-	-	5594														0.3%	-12.3	-11.9	-14.4
Benzene, C9-13-alkyl derivs., distn. residues, sulfonated, calciur	307-593-8	97675-24-6	97675246	-	-	5595														0.3%	-12.3	-12.0	-14.4
Ethylbenzene, manuf. of, distn. residues, distn. lights.	700-371-5	178535-25-6	178535256	-	-	5596														0.3%	-12.7	-12.4	-14.8
Benzene, mono-C10-14-alkyl derivs., fractionation bottoms, int	285-597-8	85117-47-1	85117471	-	-	5597														0.3%	-13.6	-13.3	-15.7

Pharmaceuticals

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
count							*388*	*358*	*358*	*358*	*356*	*268*	*234*	*358*	*358*	*358*	*397*	*0*	*397*	*397*	*392*	*392*	*392*
sum																	*2.5E+04*		*1.9E+03*	*7%*			
standard deviation																					*2.0*	*2.1*	*2.3*
2.5-p																	*7.6E-05*		*9.3E-07*	*1%*	*-16.3*	*-16.4*	*-18.9*
50-p																	*8.2E-01*		*2.8E-02*	*4%*	*-11.6*	*-11.6*	*-13.6*
97.5-p																	*2.7E+02*		*1.7E+01*	*12%*	*-8.5*	*-8.3*	*-9.7*
Paracetamol		103-90-2	103902	165	Reach_616	5599	151	119.9	2.6E-04	8.1E+03	1.9E+00	10.2	12	2.9E-09	1.1E-07	3.5E-07				12%	-6.6	-6.4	-7.4
Metformin Hydrochloride (Metformin)		657-24-9	657249	79	PharmaBeta_488	5600	129	74.5	1.0E-02	4.4E+04	2.3E-03		2.1	1.3E-07	1.1E-07	3.5E-07				6%	-7.1	-7.1	-8.8
Phenobarbital		50-06-6	50066	4945	PharmaBeta_244	5601	232	244.7	1.8E-09	3.4E+03	2.1E+01	7.5		3.5E-07	1.1E-07	3.5E-07				3%	-7.6	-7.6	-9.7
Naproxen		22204-53-1	22204531	539	PharmaBeta_529	5602	230	137.6	1.7E-04	2.8E+02	1.3E+03	4.36		8.0E-09	1.1E-07	3.5E-07				12%	-7.8	-7.6	-8.8
Ibuprofen		15687-27-1	15687271	493	Reach_2393	5603	206	94.2	2.5E-02	2.8E+01	6.2E+03	4.3		1.7E-08	1.1E-07	3.5E-07				11%	-7.9	-7.7	-9.0
Gabapentin		604-75-1	604751	72	PharmaBeta_286	5604	171	300.5	3.9E-08	2.0E+03	4.3E-02	3.8	3.28	3.1E-08	3.5E-07	1.1E-06				10%	-7.8	-7.7	-9.1
Carbamazepine		298-46-4	298464	45	PharmaBeta_372	5605	236	162.4	1.2E-05	1.5E+01	1.8E+02	14.3	13.9	2.5E-08	3.5E-08	1.1E-07				10%	-8.3	-8.1	-9.4
Tramadol Hydrochloride		27203-92-5	27203925	41	PharmaBeta_757	5606	263	115.2	6.1E-05	1.4E+03	1.0E+03	14.2	4.76	3.6E-08	3.5E-07	1.1E-06				10%	-8.4	-8.2	-9.6
Amoxicillin		26787-78-0	26787780	574	Reach_2594	5607	365	329.9	6.3E-15	2.1E+04	9.3E+00	2.36	5	2.1E-07	3.5E-07	1.1E-06				5%	-8.3	-8.2	-10.2
RANITIDINE		66357-35-5	66357355	789	Reach_2879	5608	314	168.5	1.9E-04	8.0E+03	1.9E+00		6	6.2E-08	1.1E-07	3.5E-07				8%	-8.4	-8.3	-9.8
Diclofenac		15307-86-5	15307865	31	Reach_2382	5609	296	174.6	8.2E-06	1.6E+01	1.0E+04	4.35		2.2E-09	1.1E-07	1.1E-07				12%	-8.5	-8.4	-9.5
Furosemide		54-31-9	54319	62	PharmaBeta_284	5610	331	211.6	4.1E-09	5.5E+01	2.1E+02	3.5		1.9E-08	1.1E-07	3.5E-07				11%	-8.6	-8.4	-9.7
Omeprazole		73590-58-6	73590586	832	PharmaBeta_573	5611	345	254.4	1.3E-13	1.4E+01	2.9E+03	8.74	10	3.5E-08	1.1E-07	3.5E-07				10%	-8.7	-8.5	-9.9
Phenoxymethylpenicillin (Penicillin V)		87-08-01	870801	-	-	5612														6%	-8.7	-8.5	-10.3
Valproic Acid		202409-33-4	202409334	2256	PharmaBeta_231	5613	359	221.0	1.0E-08	1.6E+00	8.1E+02		11.2	3.5E-08	1.1E-08	1.1E-08				10%	-8.6	-8.5	-9.9
Cholestyramine		11041-12-6	11041126	-	-	5614														6%	-8.8	-8.6	-10.4
Lamotrigine		84057-84-1	84057841	102	PharmaBeta_428	5615	256	189.2	1.3E-06	4.4E+02	9.8E+00		8.54	2.2E-09	3.5E-08	1.1E-07				12%	-8.8	-8.6	-9.6
Sulfamethoxazol		723-46-6	723466	86	PharmaBeta_703	5616	253	172.4	1.7E-05	1.3E+03	3.0E+00	5.68	12.2	1.3E-07	1.1E-07	1.1E-06				6%	-8.8	-8.6	-10.4
Mebeverine Hydrochloride		2753-45-9	2753459	6362	PharmaUBA	5617	466													6%	-8.9	-8.7	-10.5
Theophylline		65807-02-5	65807025	730	Reach_47	5618	180	193.3	7.4E-08	9.3E+04	4.1E-01	8.7		7.0E-09	1.1E-07	3.5E-07				12%	-8.8	-8.7	-9.8
STRONTIUM		165800-03-3	165800033	504	PharmaBeta_452	5619	337	221.7	9.2E-09	1.4E+03	1.8E+01	14.8	11	4.4E-08	1.1E-07	3.5E-07				9%	-8.9	-8.8	-10.2
flucloxacillin		5250-39-5	5250395	3062	PharmaBeta_260	5620	454	289.6	2.2E-13	4.5E+00	2.6E+03	2.47		3.5E-07	3.5E-08	3.5E-07				4%	-8.9	-8.8	-11.0
PROPRANOLOL HYDROCHLORIDE		7722-84-1	7722841	6452	PharmaBeta_779	5621	34													6%	-9.1	-8.8	-10.6
Diltiazem Hydrochloride （Diltiazem）		42399-41-7	42399417	637	PharmaBeta_173	5622	415	231.5	4.0E-09	6.6E+00	6.2E+02		6	1.9E-07	1.1E-07	3.5E-07				5%	-9.0	-8.8	-10.8
Oxytetracycline		79-57-2	79572	923	PharmaBeta_583	5623	460	344.2	1.2E-20	6.6E+03	1.3E-03	3.28	5	1.7E-07	3.5E-07	1.1E-06				5%	-8.8	-8.9	-10.7
Thiamine Hydrochloride		59467-70-8	59467708	736	PharmaBeta_502	5624	326	200.7	6.8E-07	6.7E+01	2.1E+04		8	3.4E-08	1.1E-08	1.1E-08				11%	-9.0	-8.9	-10.3
Allopurinol		315-30-0	315300	2628	PharmaBeta_24	5625	136	164.2	5.0E-05	8.7E+04	7.2E-02	9.3		3.5E-07	1.1E-07	3.5E-07				3%	-8.8	-8.9	-11.1
Bezafibrate		41859-67-0	41859670	53	PharmaBeta_89	5626	362	230.4	8.2E-09	6.5E-01	1.8E+04	3.99	15	9.2E-08	1.1E-07	1.1E-06				8%	-9.0	-8.9	-10.6
Simvastatin		79902-63-9	79902639	927	PharmaBeta_689	5627	419	206.8	5.6E-10	8.3E-01	1.5E+05	14.6		1.5E-07	1.1E-07	3.5E-07				9%	-8.8	-8.9	-10.8
Clopidogrel		113665-84-2	113665842	8	PharmaBeta_405	5628	322	158.3	3.9E-05	4.9E+01	6.6E+03		13.7	7.3E-08	1.1E-07	3.5E-07				9%	-9.1	-8.9	-10.6
Erythromycin		114-07-8	114078	336	Reach_933	5629	734	349.8	2.8E-23	2.2E+00	3.0E+02	12.7	5	2.7E-07	1.1E-07	3.5E-07				4%	-9.1	-9.0	-11.0
Atenolol		298-46-4	298464	44	PharmaBeta_58	5630	266	183.9	1.0E-07	1.5E+04	9.3E-01	13.8	4.51	2.9E-07	1.1E-07	3.5E-07				4%	-8.8	-9.0	-11.0
Cefalexin		15686-71-2	15686712	492	PharmaBeta_117	5631	347	326.8	4.3E-13	3.4E+02	9.8E-01	2.75	7	4.7E-08	3.5E-07	1.1E-06				9%	-9.1	-9.0	-10.4
VERAPAMIL HYDROCHLORIDE		119478-56-7	119478567	5622	PharmaBeta_483	5632	438													6%	-9.3	-9.0	-10.8
Amitriptyline		54024-22-5	54024225	662	Reach_8	5633	277	134.4	4.8E-05	3.5E+00	8.9E+04		5	2.3E-08	1.1E-08	3.5E-08				11%	-9.2	-9.0	-10.4
Sertraline		79617-96-2	79617962	924	PharmaBeta_684	5634	306	139.7	1.6E-04	7.5E-01	1.9E+05		5	2.9E-08	3.5E-09	1.1E-08				12%	-9.2	-9.0	-10.4
MORPHINE		57-27-2	57272	721	PharmaBeta_518	5635	285	173.8	2.5E-08	1.3E+04	5.2E+00	9.66	6	1.7E-08	1.1E-07	3.5E-07				11%	-9.2	-9.1	-10.3
Hydroxychloroquine Sulphate		16679-58-6	16679586	6397	PharmaBeta_159	5636	1069													6%	-9.3	-9.1	-10.9
Trimethoprim		738-70-5	738705	89	PharmaBeta_765	5637	290	188.9	1.0E-06	7.5E+02	5.4E+00		6.96	1.4E-07	1.1E-07	3.5E-07				6%	-9.2	-9.1	-10.9
Clarithromycin		81103-11-9	81103119	99	PharmaBeta_391	5638	748	349.8	3.1E-23	7.7E-01	1.5E+03	12.7	5.45	2.3E-07	1.1E-07	1.1E-06				5%	-9.3	-9.2	-11.2
Celecoxib		169590-42-5	169590425	508	PharmaBeta_124	5639	381	212.6	1.6E-07	2.4E+00	3.0E+03	10	15	3.1E-09	3.5E-08	3.5E-08				12%	-9.3	-9.2	-10.2
Hydrochlorothiazide		58-93-5	58935	69	PharmaBeta_318	5640	298	202.3	2.4E-08	1.1E+03	7.9E-01	8.88		2.0E-08	1.1E-07	3.5E-07				11%	-9.3	-9.2	-10.5
Aspirin		50-78-2	50782	666	Reach_9	5641	180	93.1	8.7E-03	2.3E+03	1.3E+01	3.5		1.1E-06	3.5E-07	1.1E-06				2%	-9.4	-9.2	-11.7
Ursodeoxycholic Acid		214766-78-6	214766786	6424	PharmaBeta_156	5642	1632													6%	-9.5	-9.3	-11.1
Irbesartan		138402-11-6	138402116	444	PharmaBeta_343	5643	429	291.5	1.6E-13	4.3E-04	2.0E+05	3.63	4	1.1E-07	3.5E-08	1.1E-07				10%	-9.2	-9.3	-11.0
Sitagliptin		486460-32-6	486460326	2974	Reach_4660	5644	407	181.6	3.9E-06	5.6E+00	2.5E+01		5.39	1.1E-07	3.5E-08	1.1E-07				7%	-9.4	-9.3	-11.0
Ketoprofen		22071-15-4	22071154	38	PharmaBeta_384	5645	254	149.2	1.9E-04	1.3E+01	1.0E+03	4.07		3.6E-09	1.1E-07	3.5E-07				12%	-9.6	-9.3	-10.4
Etodolac		120287-85-6	120287856	6418	PharmaBeta_126	5646	1431													6%	-9.5	-9.3	-11.1
Cimetidine		51481-61-9	51481619	1129	PharmaUBA	5647	252	194.2	7.3E-07	3.4E+03	3.7E+00	12.2	7	8.9E-08	3.5E-08	3.5E-07				7%	-9.4	-9.3	-11.0
Mefenamic Acid		61-68-7	61687	1150	PharmaUBA	5648	241	152.8	7.8E-06	1.1E+01	1.9E+05	4.3	16	1.3E-08	1.1E-07	3.5E-07				12%	-9.2	-9.3	-10.8
Valsartan		137862-53-4	137862534	442	PharmaBeta_775	5649	436	294.1	1.1E-13	1.3E-02	4.5E+03	3.09		1.6E-07	3.5E-08	1.1E-07				6%	-9.5	-9.3	-11.2
Sucralfate		39474-58-3	39474583	6377	PharmaUBA	5650	1559													6%	-9.6	-9.4	-11.2
Flutamide		13311-84-7	13311847	427	PharmaBeta_270	5651	276	154.9	1.5E-04	3.1E+00	3.2E+03	12.3		2.2E-09	3.5E-08	1.1E-07				12%	-9.7	-9.4	-10.5
Lansoprazole		103577-45-3	103577453	1372	PharmaBeta_430	5652	369	240.4	1.7E-12	7.8E-01	4.1E+03	8.79	10.1	3.5E-07	1.1E-07	3.5E-07				4%	-9.5	-9.4	-11.6
Mirtazapine		61337-67-5	61337675	-	-	5653														6%	-9.7	-9.5	-11.3
Amlodipine		88150-42-9	88150429	982	PharmaBeta_42	5654	409	200.6	1.6E-07	1.5E+03	1.2E+02		5	1.9E-07	1.1E-07	3.5E-07				5%	-9.6	-9.5	-11.4
Nifedipine		21829-25-4	21829254	1102	PharmaBeta_549	5655	346	176.5	3.5E-06	1.1E+01	3.2E+02		12	1.1E-07	1.1E-07	3.5E-07				7%	-9.7	-9.5	-11.2
Lidocaine		137-58-6	137586	26	PharmaBeta_451	5656	234	144.2	9.0E-04	6.8E+02	4.6E+01	13.1	6.1	3.9E-08	3.5E-08	1.1E-07				10%	-9.7	-9.5	-10.9
MYCOPHENOLATE		139264-17-8	139264178	1918	PharmaBeta_800	5657	287	201.7	1.9E-07	1.5E+03	8.3E+01	12	5.3	3.5E-07	3.5E-08	1.1E-07				3%	-9.4	-9.5	-11.6
Codeine Phosphate (Codeine)		76-57-3	76573	3719	PharmaBeta_416	5658	299	168.6	2.5E-08	8.8E+02	1.9E+01	14.1	5.79	1.1E-06	1.1E-07	3.5E-07				2%	-9.2	-9.5	-12.0
Sulfasalazine		599-79-1	599791	3300	PharmaBeta_704	5659	398	264.6	3.0E-12	8.2E-03	6.5E+03	1.84	11.3	1.1E-06	3.5E-07	1.1E-06				3%	-9.5	-9.6	-12.0
Miconazole		22916-47-8	22916478	5364	PharmaUBA	5660	416	215.6	2.4E-08	2.4E-02	1.8E+06		7.54	3.5E-09	3.5E-09	3.5E-09				13%	-9.5	-9.6	-10.8
Nitrofurantoin		67-20-9	67209	791	PharmaBeta_557	5661	238	212.6	9.1E-09	9.9E+01	6.8E-01	7.24		1.5E-07	1.1E-07	3.5E-07				6%	-9.6	-9.6	-11.4
Docusate Sodium		198904-31-3	198904313	2244	PharmaBeta_57	5662	705	349.8	1.4E-24	1.1E-02	7.6E+02	8.78	10.1	3.5E-07	1.1E-07	3.5E-07				4%	-9.7	-9.6	-11.8
Ketoconazole		65277-42-1	65277421	78	PharmaBeta_383	5663	531	291.8	8.5E-12	2.6E-01	2.8E+04		7.6	2.3E-08	3.5E-08	1.1E-07				11%	-9.7	-9.6	-11.0
Gliclazide		29110-47-2	29110472	5323	PharmaUBA	5664	323	207.5	1.6E-07	2.3E+02	1.3E+02	6	10.6	1.1E-06	1.1E-07	3.5E-07				2%	-9.5	-9.7	-12.2
Betamethasone		378-44-9	378449	619	Reach_1261	5665	392	216.8	7.7E-12	6.5E+01	5.2E+01	13		1.0E-07	3.5E-07	1.1E-06				7%	-9.9	-9.7	-11.4
Quinine		130-95-0	130950	5427	PharmaUBA	5666	324	189.5	1.3E-08	4.1E+02	1.9E+03	11.8	5.43	1.1E-06	1.1E-07	3.5E-07				2%	-9.7	-9.7	-12.2
Temazepam		147127-20-6	147127206	5457	PharmaUBA	5667	301	198.9	2.3E-08	6.3E+01	1.4E+02	13.7	12.2	3.5E-08	1.1E-08	3.5E-08				10%	-9.9	-9.7	-11.1

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Calcium Acetate		1492-18-8	1492188	6274	PharmaBeta_363	5668	158													6%	-10.0	-9.8	-11.6
Diazepam		439-14-5	439145	640	PharmaBeta_166	5669	285	181.9	1.4E-05	3.2E+01	5.0E+02		11	3.5E-08	1.1E-08	3.5E-08				10%	-10.0	-9.8	-11.2
Amantadine Hydrochloride		66592-87-8	66592878	5982	PharmaBeta_116	5670	381													6%	-10.0	-9.8	-11.6
Prednisolone		50-24-8	50248	656	Reach_6	5671	360	215.3	9.1E-12	4.4E+02	2.5E+01	13.2		1.4E-07	3.5E-07	1.1E-06				6%	-10.0	-9.8	-11.7
FLUOXETINE		54910-89-3	54910893	692	PharmaBeta_268	5672	309	105.3	3.4E-03	4.8E+01	4.5E+04		4	2.2E-07	1.1E-07	3.5E-07				7%	-10.0	-9.9	-11.9
Atorvastatin		134523-00-5	134523005	431	PharmaBeta_60	5673	559	349.8	9.3E-23	3.0E-03	2.3E+06	4.34	16	1.9E-07	1.1E-08	3.5E-08				11%	-9.7	-9.9	-11.7
Oxazepam		604-75-1	604751	73	PharmaBeta_579	5674	287	208.7	5.5E-10	8.8E+01	2.1E+02	11.5	12.2	2.2E-08	1.1E-08	3.5E-08				11%	-10.0	-9.9	-11.2
Dipyridamole		58-32-2	58322	3243	PharmaBeta_178	5675	505	319.4	1.6E-18	1.9E+00	5.5E+02	15.3	7.51	1.1E-06	1.1E-07	3.5E-07				2%	-9.8	-9.9	-12.4
Cefadroxil		66592-87-8	66592878	5982	PharmaBeta_116	5676	381													6%	-10.1	-9.9	-11.7
Fluconazole		86386-73-4	86386734	970	PharmaBeta_261	5677	306	170.6	3.9E-07	3.6E+03	1.8E+00	14.5	12	2.2E-09	3.5E-07	1.1E-06				12%	-10.2	-10.0	-11.0
Hydrocortisone		50-23-7	50237	655	Reach_5	5678	362	214.5	1.6E-11	4.7E+02	4.2E+01	13.2		2.1E-07	1.1E-07	3.5E-07				5%	-10.1	-10.0	-12.0
Tetracycline		60-54-8	60548	754	PharmaBeta_731	5679	444	327.2	2.8E-19	2.6E+03	4.7E-02	3.36	5	1.7E-07	3.5E-07	1.1E-06				5%	-10.0	-10.0	-11.9
Tranexamic Acid		274901-16-5	274901165	2510	PharmaBeta_786	5680	303	190.3	1.3E-08	1.1E+02	6.2E+00	15.4	6.41	1.1E-06	1.1E-07	3.5E-07				1%	-9.7	-10.1	-12.6
Aciclovir		51-52-5	51525	5108	PharmaBeta_637	5681	170	164.8	9.2E-06	9.6E+02	9.5E+00	7.5		1.1E-06	3.5E-07	1.1E-06				1%	-10.0	-10.1	-12.6
Felodipine		72519-76-3	72519763	-	-	5682														6%	-10.3	-10.1	-11.9
Mesalazine (Systemic)		89-57-6	89576	3980	Reach_345	5683	153	128.9	8.1E-06	1.4E+04	9.5E+00	2.4	8.2	3.5E-06	3.5E-07	1.1E-06				1%	-9.6	-10.1	-12.6
Fenofibrate		49562-28-9	49562289	649	Reach_2761	5684	361	157.7	8.3E-05	5.3E-02	1.5E+05			6.0E-08	1.1E-07	1.1E-06				10%	-10.2	-10.1	-11.7
Timolol		26839-75-8	26839758	2488	PharmaBeta_740	5685	316	176.4	7.3E-08	9.8E+03	5.6E+01	14.1	4.21	1.1E-06	3.5E-07	1.1E-06				2%	-10.0	-10.1	-12.6
Isoniazid		54910-89-3	54910893	691	PharmaBeta_346	5686	137	119.0	1.6E-03	3.2E+05	1.5E-01		10	9.1E-09	3.5E-08	1.1E-07				12%	-10.3	-10.1	-11.2
Losartan Potassium		5633-20-5	5633205	3190	PharmaBeta_585	5687	358	185.8	2.3E-08	1.4E+01	9.1E+03	11.5	5.74	1.1E-06	1.1E-07	3.5E-07				3%	-10.1	-10.1	-12.6
Methocarbamol		61-32-5	61325	5360	PharmaUBA	5688	241	120.5	9.1E-05	1.1E+04	5.5E-01	11.6		1.1E-06	1.1E-07	3.5E-07				1%	-9.8	-10.2	-12.7
Dihydrocodeine		125-28-0	125280	5283	PharmaUBA	5689	301	167.9	2.7E-07	4.5E+02	3.1E+01	14.6	5.79	1.1E-06	1.1E-07	3.5E-07				2%	-10.0	-10.2	-12.7
Venlafaxine		58-46-8	58468	5154	PharmaBeta_730	5690	317	157.8	7.1E-05	1.7E+01	4.6E+02		7.02	1.1E-06	1.1E-07	3.5E-07				2%	-10.3	-10.2	-12.7
Primidone		125-33-7	125337	5420	PharmaUBA	5691	218	195.6	4.4E-08	2.9E+03	5.4E+00	11.8		3.5E-07	1.1E-07	3.5E-07				3%	-10.1	-10.2	-12.3
Balsalazide Sodium		38304-91-5	38304915	2820	PharmaBeta_508	5692	209	173.1	1.8E-06	2.8E+04	2.2E+01		9.4	1.1E-06	3.5E-08	1.1E-07				2%	-9.8	-10.2	-12.7
Disulfiram		97-77-8	97778	1060	Reach_487	5693	297	138.9	8.8E-04	9.7E+00	4.7E+03		16	2.7E-08	3.5E-07	1.1E-06				11%	-10.4	-10.2	-11.6
Nitrazepam		146-22-5	146225	474	PharmaBeta_556	5694	281	209.0	4.1E-08	1.3E+02	2.8E+02	10.8	11	5.4E-08	1.1E-07	3.5E-07				9%	-10.4	-10.2	-11.7
Levodopa		59-92-7	59927	745	PharmaBeta_444	5695	197	295.2	3.4E-08	7.1E+05	5.8E-03	2.35	5	7.9E-07	3.5E-07	1.1E-06				2%	-9.9	-10.2	-12.7
Acetylcysteine		616-91-1	616911	3348	PharmaBeta_5	5696	163	131.3	1.5E-03	1.9E+05	2.2E-01	3.03		1.1E-06	3.5E-07	3.5E-07				1%	-9.9	-10.2	-12.8
Fexofenadine Hydrochloride		93-14-1	93141	4061	PharmaBeta_312	5697	198	100.0	3.4E-04	1.2E+05	2.6E+00	14		1.1E-06	1.1E-07	3.5E-07				1%	-9.9	-10.2	-12.8
Azithromycin		83905-01-5	83905015	957	Reach_4465	5698	749	349.8	3.5E-22	7.4E-01	1.7E+03	12.6	5	2.6E-07	3.5E-07	1.1E-06				5%	-10.4	-10.3	-12.3
Quetiapine		143322-58-1	143322581	1963	PharmaBeta_199	5699	383	234.2	1.4E-09	1.2E+01	3.2E+03		4.83	1.1E-06	3.5E-08	1.1E-07				2%	-10.2	-10.3	-12.8
Lymecycline		158966-92-8	158966928	2066	PharmaBeta_517	5700	586	320.7	5.5E-19	2.8E-05	3.3E+09	4.73	10.6	3.5E-07	3.5E-08	1.1E-07				13%	-10.3	-10.3	-11.2
Carbocisteine		638-23-3	638233	5239	PharmaUBA	5701	179	259.0	2.0E-05	3.3E+04	5.8E-05	1.89	5.31	3.5E-06	3.5E-07	1.1E-06				1%	-9.5	-10.3	-12.8
Cinnarizine		298-57-5	298575	-	-	5702														6%	-10.5	-10.3	-12.1
Nicotinic Acid		59-67-6	59676	739	Reach_52	5703	123	63.3	1.2E-02	4.1E+04	4.9E+00	1.96	9	6.3E-07	1.1E-07	3.5E-07				2%	-10.2	-10.3	-12.7
Oxycodone		76-42-6	76426	3711	PharmaBeta_581	5704	315	179.3	3.0E-08	1.4E+04	4.6E+00	13.6	5.94	3.5E-07	1.1E-07	3.5E-07				3%	-10.2	-10.3	-12.5
Etoricoxib		202409-33-4	202409334	2256	PharmaBeta_231	5705	359	221.0	1.0E-08	1.6E+00	8.1E+02		11.2	3.5E-08	1.1E-08	1.1E-08				10%	-10.4	-10.3	-11.7
Disopyramide		3737-09-5	3737095	115	PharmaBeta_179	5706	339	202.2	2.8E-06	1.4E+01	9.1E+02	12.8	5	4.0E-08	1.1E-07	3.5E-07				10%	-10.6	-10.3	-11.8
Finasteride		98319-26-7	98319267	1070	PharmaBeta_253	5707	373	236.2	6.4E-10	1.2E-02	1.6E+03	14.8	14	8.2E-08	1.1E-07	3.5E-07				8%	-10.6	-10.4	-12.0
Captopril		62571-86-2	62571862	1103	PharmaUBA	5708	217	133.8	9.7E-04	1.4E+04	6.9E+00	3.25		1.2E-07	3.5E-07	1.1E-06				6%	-10.6	-10.4	-12.1
Gemfibrozil		25812-30-0	25812300	570	PharmaBeta_299	5709	250	129.0	4.1E-03	3.0E+01	5.9E+04	4.81		3.5E-09	3.5E-07	1.1E-06				12%	-10.3	-10.4	-11.7
Zopiclone		43200-80-2	43200802	2908	PharmaBeta_803	5710	389	228.4	1.3E-08	8.4E+02	3.5E+01		7.2	3.5E-07	3.5E-08	1.1E-07				3%	-10.3	-10.4	-12.6
Crotamiton		3546-03-0	3546030	5266	PharmaUBA	5711	203	94.0	6.5E-02	1.1E+02	5.4E+02		14.4	3.5E-07	1.1E-07	3.5E-07				4%	-10.7	-10.4	-12.5
Phenytoin		57-41-0	57410	3229	PharmaBeta_250	5712	252	218.1	1.8E-09	4.9E+01	1.4E+02	8.3		1.1E-06	1.1E-07	3.5E-07				2%	-10.3	-10.4	-12.9
Indometacin		21829-25-4	21829254	1101	PharmaBeta_338	5713	358	219.4	6.8E-08	2.3E+00	1.7E+04	4.49		1.6E-07	1.1E-07	3.5E-07				7%	-10.5	-10.5	-12.3
Urea		57-13-6	57136	719	Reach_39	5714	60	29.0	2.8E+01	4.2E+05	2.8E-02	14.3	14	7.0E-07	3.5E-07	1.1E-06				2%	-10.7	-10.5	-12.9
Levetiracetam		27262-47-1	27262471	5007	PharmaBeta_442	5715	170	140.8	4.7E-04	1.5E+05	3.2E-01	13.6	15.3	3.5E-06	1.1E-06	3.5E-06				1%	-10.1	-10.5	-13.0
Carvedilol		72956-09-3	72956093	826	PharmaBeta_379	5716	406	252.1	7.9E-12	1.8E+00	1.1E+03	14	6	1.6E-07	3.5E-08	1.1E-07				6%	-10.6	-10.5	-12.3
Acamprosate Calcium		55-98-1	55981	708	PharmaBeta_110	5717	246	129.8	1.2E-05	1.5E+04	2.1E-01			1.1E-06	3.5E-07	1.1E-06				1%	-10.2	-10.5	-13.0
Meloxicam		71125-39-8	71125398	-	-	5718														6%	-10.7	-10.5	-12.3
Hydrogen Peroxide		7722-84-1	7722841	6452	PharmaBeta_779	5719	34													6%	-10.7	-10.5	-12.3
Aminophylline		183321-74-6	183321746	2183	PharmaBeta_216	5720	393	221.6	9.4E-09	1.2E+00	6.2E+02		8.12	1.1E-06	1.1E-07	3.5E-07				2%	-10.5	-10.5	-13.0
Aminophylline		183321-74-6	183321746	2183	PharmaBeta_216	5721	393	221.6	9.4E-09	1.2E+00	6.2E+02		8.12	1.1E-06	1.1E-07	3.5E-07				2%	-10.5	-10.5	-13.0
Ergocalciferol (Vitamin D2)		78755-81-4	78755814	4957	PharmaBeta_262	5722	303	205.4	1.2E-07	2.6E+01	1.1E+01		12	1.1E-06	1.1E-07	3.5E-07				1%	-10.3	-10.5	-13.0
Carbidopa		745-65-3	745653	3640	PharmaBeta_27	5723	354	217.9	3.1E-11	3.1E+00	5.4E+03	4.9		1.1E-06	1.1E-07	3.5E-07				3%	-10.5	-10.5	-13.0
Lisinopril		83915-83-7	83915837	3852	PharmaBeta_454	5724	406	326.4	5.3E-13	2.6E+01	1.1E-01	1.92	3.53	1.1E-06	1.1E-07	3.5E-07				1%	-10.1	-10.6	-13.1
Isosorbide		53123-88-9	53123889	3089	PharmaBeta_690	5725	914	349.8	4.1E-34	4.2E-05	6.5E+04	10.4		1.1E-06	1.1E-07	3.5E-07				5%	-10.8	-10.6	-13.0
Ramipril		87333-19-5	87333195	3928	PharmaBeta_646	5726	417	318.5	5.1E-09	1.1E+00	2.1E+03	3.07	8.45	1.1E-06	1.1E-07	3.5E-07				2%	-10.6	-10.6	-13.1
Sodium Citrate		1716-12-7	1716127	6294	PharmaBeta_533	5727	215													6%	-10.8	-10.6	-12.4
CLINDAMYCIN		18323-44-9	18323449	2181	PharmaBeta_394	5728	425	255.3	7.0E-15	1.3E+02	1.0E+02	11.2	6.53	1.1E-06	1.1E-07	3.5E-07				2%	-10.5	-10.6	-13.1
Norfloxacin		70458-96-7	70458967	812	PharmaBeta_562	5729	319	314.7	1.1E-09	5.4E+02	4.9E-01	6.15	5	3.0E-08	3.5E-08	3.5E-07				10%	-10.7	-10.6	-12.0
Chlordiazepoxide		58-25-3	58253	1127	PharmaUBA	5730	300	234.1	1.3E-09	1.5E+05	2.6E+02		9	3.4E-08	3.5E-09	1.1E-08				10%	-10.7	-10.7	-12.0
Nicotine		66085-59-4	66085594	5067	PharmaBeta_551	5731	162	57.3	4.3E+00	9.1E+05	1.0E+01		5.7	3.5E-07	3.5E-08	1.1E-07				3%	-10.8	-10.7	-12.9
Ofloxacin		82419-36-1	82419361	945	PharmaBeta_568	5732	361	318.1	1.3E-10	6.3E+01	6.3E-01	6.08	6	5.2E-09	1.1E-07	3.5E-07				12%	-10.8	-10.7	-11.8
Pregabalin		148553-50-8	148553508	2003	PharmaBeta_626	5733	159	282.5	2.7E-07	3.2E+03	1.7E-02	3.8	3.28	3.5E-06	3.5E-07	1.1E-06				1%	-10.0	-10.7	-13.3
Testosterone		58-22-0	58220	67	Reach_46	5734	288	144.6	2.3E-06	2.4E+01	1.9E+03	16		3.4E-07	3.5E-08	1.1E-07				4%	-10.9	-10.8	-12.9
Sildenafil		1397-89-3	1397893	1923	PharmaBeta_688	5735	475	327.4	5.0E-16	1.7E+01	3.0E+02	7.43	7.56	3.5E-07	1.1E-07	3.5E-07				4%	-10.9	-10.8	-12.9
Chloral Hydrate		302-17-0	302170	1126	PharmaUBA	5736	165	22.2	1.2E+03	7.1E+05	9.5E+00	10.1		8.7E-08	1.1E-08	3.5E-08				7%	-11.1	-10.8	-12.4
PRAVASTATIN		53-03-2	53032	5101	PharmaBeta_623	5737	425	242.7	8.1E-14	5.1E+01	1.3E+03	4.34		1.1E-06	1.1E-07	3.5E-07				2%	-10.8	-10.8	-13.3
Sulfadiazine		68-35-9	68359	1165	PharmaUBA	5738	250	179.0	7.0E-07	1.2E+03	4.6E-01	6.48	12	4.7E-09	1.1E-07	3.5E-07				12%	-11.0	-10.8	-11.9
Lacosamide		585-86-4	585864	4999	PharmaBeta_425	5739	250	196.4	4.3E-07	9.4E+02	6.9E-01	12.1		3.5E-07	1.1E-07	3.5E-07				3%	-10.7	-10.8	-13.0
Clozapine		5786-251-0	57862510	-	-	5740														6%	-11.1	-10.8	-12.6
Rifampicin		133040-01-4	133040014	1863	PharmaBeta_656	5741	823	349.8	4.1E-32	8.8E-04	1.7E+04	3.78	5.9	3.5E-07	1.1E-07	3.5E-07				5%	-11.0	-10.8	-13.0
Oxcarbazepine		28721-07-5	28721075	2541	PharmaBeta_584	5742	252	185.2	1.0E-06	9.7E+02	1.3E+01	14.2	14.1	1.1E-06	1.1E-07	3.5E-07				1%	-10.6	-10.8	-13.4

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
TERBINAFINE		91161-71-6	91161716	4012	Reach_4498	5743	291	146.5	7.8E-05	2.0E+00	6.5E+05		6.9	1.1E-06	3.5E-08	1.1E-07				7%	-10.9	-10.8	-13.2
Demeclocycline Hydrochloride		64-73-3	64733	5969	Reach_74	5744	501													6%	-11.1	-10.9	-12.7
Sulpiride		15676-16-1	15676161	5454	PharmaUBA	5745	341	226.5	1.6E-08	2.0E+03	4.5E+00	10.3	4.82	1.1E-06	1.1E-07	3.5E-07				1%	-10.5	-10.9	-13.4
Levofloxacin		100986-85-4	100986854	139	PharmaBeta_445	5746	361	318.1	1.3E-10	6.3E+01	6.3E-01	6.08	6	5.2E-09	1.1E-07	3.5E-07				12%	-11.0	-10.9	-12.0
ZUCLOPENTHIXOL		53772-83-1	53772831	3109	PharmaBeta_804	5747	401	223.0	3.9E-11	6.4E-01	5.8E+03	14.9	6.29	1.1E-08	3.5E-09	1.1E-08				12%	-11.1	-10.9	-12.1
Abacavir		136470-78-5	136470785	1899	PharmaBeta_2	5748	286	222.7	4.2E-11	1.3E+02	4.2E+01	15.9	8.93	1.1E-06	3.5E-07	1.1E-06				2%	-10.8	-10.9	-13.4
FLUVASTATIN		93957-54-1	93957541	4094	PharmaBeta_272	5749	411	255.8	2.5E-14	7.3E-01	7.1E+04	4.34		1.1E-07	1.1E-08	3.5E-08				9%	-11.0	-10.9	-12.7
Ampicillin		69-53-4	69534	808	Reach_94	5750	349	324.9	3.8E-11	3.5E+03	2.8E+01	2.35	7	5.5E-08	1.1E-07	3.5E-07				9%	-11.1	-10.9	-12.5
Methotrexate		59-05-2	59052	732	PharmaBeta_492	5751	454	345.0	2.0E-15	1.7E+02	5.2E-02	3.24	8	5.6E-08	1.1E-07	3.5E-07				9%	-11.0	-11.0	-12.5
Clotrimazole		23593-75-1	23593751	553	PharmaBeta_413	5752	345	206.6	2.8E-07	9.4E-02	1.8E+06		7	2.0E-08	3.5E-08	3.5E-08				12%	-10.7	-11.0	-12.5
Progesterone		57-83-0	57830	65	Reach_43	5753	314	149.8	3.6E-04	4.0E+01	4.7E+03			3.4E-07	3.5E-08	1.1E-07				4%	-11.2	-11.0	-13.1
Nortriptyline		67018-85-3	67018853	5392	PharmaUBA	5754	263	129.8	2.9E-04	6.2E+00	5.5E+04		4.1	3.5E-07	1.1E-08	3.5E-08				6%	-11.2	-11.0	-13.1
Triamterene		396-01-1	396011	-	-	5755														6%	-11.2	-11.0	-12.8
Indapamide		26807-65-8	26807658	5332	PharmaUBA	5756	366	240.9	4.2E-09	7.3E+01	4.6E+02	9.7		1.1E-07	3.5E-08	1.1E-07				7%	-11.2	-11.0	-12.8
Fluorouracil		51333-22-3	51333223	669	PharmaBeta_104	5757	431	234.0	1.5E-12	2.2E+00	4.1E+02	13.3		4.0E-08	3.5E-07	1.1E-06				10%	-11.3	-11.1	-12.5
Methylprednisolone		83-43-2	83432	3846	PharmaBeta_498	5758	374	219.1	5.9E-12	8.9E+01	6.6E+01	13.2		1.1E-06	3.5E-07	1.1E-06				2%	-11.0	-11.1	-13.6
Citalopram Hydrobromide (Citalopram)		72559-06-9	72559069	3606	PharmaBeta_655	5759	847	349.8	1.2E-31	1.1E-04	3.2E+07	7.16	4.36	1.1E-06	1.1E-07	3.5E-07				10%	-10.7	-11.1	-12.7
Domperidone		57808-66-9	57808669	5289	PharmaUBA	5760	426	277.5	4.1E-12	1.6E-01	2.2E+03	10.2	5.83	1.1E-06	3.5E-08	1.1E-07				2%	-11.0	-11.1	-13.6
GLYCEROL		56-81-5	56815	716	Reach_30	5761	92	19.4	1.1E-02	1.0E+06	2.2E-02	14.2		1.2E-06	1.1E-06	3.5E-06				1%	-10.9	-11.1	-13.6
Medroxyprogesterone Acetate		4928-02-3	4928023	5213	PharmaUBA	5762	387	188.2	8.9E-07	2.8E+00	1.2E+04			3.5E-07	3.5E-08	1.1E-07				5%	-11.3	-11.1	-13.3
DULOXETINE		116539-59-4	116539594	1652	PharmaBeta_193	5763	297	157.0	1.6E-05	1.1E-01	4.8E+04		4.4	1.1E-06	3.5E-08	1.1E-07				4%	-11.4	-11.1	-13.6
Nadolol		1404-04-2	1404042	1154	PharmaUBA	5764	309	181.3	1.3E-08	1.0E+03	1.5E+01	13.8	4	3.7E-08	1.1E-07	3.5E-07				10%	-11.3	-11.1	-12.5
Mebendazole		31431-39-7	31431397	599	PharmaBeta_470	5765	295	223.4	1.1E-09	4.0E+01	5.1E+02	9.97	10	6.5E-09	1.1E-07	3.5E-07				12%	-11.4	-11.1	-12.3
Budesonide		51333-22-3	51333223	669	PharmaBeta_104	5766	431	234.0	1.5E-12	2.2E+00	4.1E+02	13.3		4.0E-08	3.5E-07	1.1E-06				10%	-11.4	-11.2	-12.6
Famotidine		76824-35-6	76824356	1100	PharmaBeta_239	5767	337	222.6	3.9E-08	7.4E+03	2.2E-01	11.2	7	3.9E-08	3.5E-07	1.1E-06				10%	-11.3	-11.2	-12.6
Sodium Benzoate		532-32-1	532321	1218	Reach_1329	5768	144													6%	-11.4	-11.2	-13.0
Imipramine		50-49-7	50497	5330	PharmaUBA	5769	280	140.9	8.5E-05	1.0E+01	1.0E+05		4.8	3.5E-07	1.1E-08	3.5E-08				7%	-11.4	-11.2	-13.3
Hyoscine Hydrobromide		114-49-8	114498	5612	Reach_934	5770	384													6%	-11.4	-11.2	-13.0
Nevirapine		129618-40-2	129618402	1829	PharmaBeta_548	5771	266	196.1	4.5E-07	2.3E+01	7.8E+03	14.8	10	3.5E-07	3.5E-08	1.1E-07				5%	-11.3	-11.2	-13.4
DOXAZOSIN		74191-85-8	74191858	3633	PharmaBeta_187	5772	451	274.6	2.4E-12	2.8E+00	1.2E+02		6.58	1.1E-06	3.5E-08	1.1E-07				2%	-10.9	-11.2	-13.7
MEMANTINE		19982-08-2	19982082	2246	PharmaBeta_480	5773	179	54.6	2.5E-02	2.1E+01	2.2E+03		3.5	3.5E-07	3.5E-08	1.1E-07				4%	-11.5	-11.2	-13.3
Pantoprazole		102625-70-7	102625707	1349	PharmaBeta_592	5774	383	253.3	1.6E-13	8.8E+00	1.4E+02	8.45	10.1	1.1E-06	1.1E-07	3.5E-07				2%	-11.1	-11.2	-13.8
TAMOXIFEN		10540-29-1	10540291	174	Reach_2294	5775	372	180.9	4.6E-06	8.6E-03	2.0E+06		6	1.6E-08	3.5E-08	1.1E-07				12%	-11.1	-11.3	-12.8
Orlistat		96-88-8	96888	4154	PharmaBeta_576	5776	496	264.0	1.3E-11	1.1E-03	1.5E+08	13.1	15.9	1.1E-06	1.1E-07	3.5E-07				11%	-10.9	-11.3	-12.6
Flurbiprofen		23155-02-4	23155024	5319	PharmaUBA	5777	244	133.9	4.7E-04	8.0E+00	6.5E+03	4.13		3.5E-07	3.5E-08	3.5E-08				5%	-11.6	-11.3	-13.5
Pentoxifylline		6493-05-6	6493056	5409	PharmaUBA	5778	278	218.0	1.6E-08	2.5E+04	3.6E+00			1.1E-06	3.5E-07	1.1E-06				1%	-11.1	-11.3	-13.8
Diethylamine Salicylate （Diethylamine）		142217-69-4	142217694	4922	PharmaBeta_205	5779	277	265.5	4.0E-15	1.3E+05	6.2E-02	9.34	10.9	3.5E-06	1.1E-06	3.5E-06				1%	-10.8	-11.3	-13.8
Risperidone		106266-06-2	106266062	188	PharmaBeta_660	5780	411	235.9	6.2E-09	8.4E-01	3.1E+03		6	1.2E-08	1.1E-07	3.5E-07				12%	-11.5	-11.3	-12.6
Itraconazole		84625-61-6	84625616	3872	PharmaBeta_351	5781	706	349.8	3.5E-18	1.3E-04	1.4E+06		8.47	1.1E-07	3.5E-08	1.1E-07				11%	-11.1	-11.3	-13.1
Calcium Gluconate		471-34-1	471341	6276	PharmaBeta_365	5782	430													6%	-11.6	-11.4	-13.2
Fluocinolone Acetonide		67-73-2	67732	1142	PharmaUBA	5783	452	222.4	4.0E-12	2.2E+01	3.6E+02	13.2		1.2E-07	1.1E-07	3.5E-07				6%	-11.6	-11.5	-13.2
Modafinil		68693-11-8	68693118	3525	PharmaBeta_514	5784	273	202.3	1.0E-09	9.7E+01	2.8E+02	12.5		1.1E-06	1.1E-07	3.5E-07				2%	-11.4	-11.5	-14.0
Griseofulvin		23210-56-2	23210562	1144	PharmaUBA	5785	353	189.1	5.5E-07	8.5E+01	8.3E+01			3.2E-07	1.1E-07	3.5E-07				4%	-11.6	-11.5	-13.6
Ezetimibe		163222-33-1	163222331	2088	PharmaBeta_237	5786	409	239.6	2.0E-12	1.3E+00	8.7E+03	10	13.4	1.1E-06	1.1E-07	3.5E-07				3%	-11.5	-11.5	-14.0
Azelaic Acid		123-99-9	123999	1782	Reach_1064	5787	188	127.2	3.1E-03	3.8E+03	5.0E+01	4.59		1.1E-06	3.5E-07	1.1E-06				2%	-11.6	-11.6	-14.1
Escitalopram		128196-01-0	128196010	1817	PharmaBeta_219	5788	324	164.0	1.5E-05	1.5E+01	5.5E+03		4.65	1.1E-06	1.1E-07	3.5E-07				3%	-11.7	-11.6	-14.1
Ropinirole		287714-41-4	287714414	5125	PharmaBeta_667	5789	260	174.6	8.4E-06	1.4E+02	1.1E+03	15.1	4.82	3.5E-07	3.5E-08	3.5E-07				4%	-11.8	-11.6	-13.8
Nilotinib		641571-10-0	641571100	3427	Reach_4930	5790	530	331.0	2.7E-16	3.5E-05	1.0E+05	14.5	8.09	1.1E-06	1.1E-07	3.5E-07				5%	-11.5	-11.6	-14.0
Aliskiren		154323-57-6	154323576	4834	PharmaBeta_23	5791	552	312.6	2.6E-18	5.2E-01	5.8E+02	13.8	4.69	1.1E-06	1.1E-07	3.5E-07				2%	-11.5	-11.6	-14.1
Linezolid		165800-03-3	165800033	504	PharmaBeta_452	5792	337	221.7	9.2E-09	1.4E+03	1.8E+01	14.8	11	4.4E-08	1.1E-07	3.5E-07				9%	-11.8	-11.6	-13.1
Telmisartan		144701-48-4	144701484	1981	PharmaBeta_719	5793	515	349.8	1.2E-17	8.6E-07	2.6E+08	3.3	7.77	3.5E-07	3.5E-08	1.1E-07				12%	-11.4	-11.6	-12.8
Olanzapine		132539-06-1	132539061	1859	PharmaBeta_570	5794	312	188.5	1.4E-06	1.3E+01	3.6E+02		6.2	1.1E-06	1.1E-07	3.5E-07				2%	-11.6	-11.6	-14.1
Dexamethasone		50-02-2	50022	652	PharmaBeta_161	5795	392	216.8	7.7E-12	6.5E+01	5.2E+01	13		1.0E-07	3.5E-07	1.1E-06				7%	-11.8	-11.6	-13.3
Cyclophosphamide		50-18-0	50180	1131	PharmaUBA	5796	261	85.7	5.9E-03	6.2E+03	9.3E+00			6.5E-09	3.5E-08	1.1E-07				12%	-11.8	-11.6	-12.7
Menthol		89-78-1	89781	994	Reach_351	5797	156	-5.9	1.0E+00	9.4E+02	2.4E+03	16		3.2E-07	1.1E-07	3.5E-07				4%	-11.9	-11.6	-13.7
Desloratadine		100643-71-8	100643718	1308	PharmaBeta_158	5798	311	180.5	4.6E-06	2.3E+00	4.3E+04		4.13	3.5E-07	3.5E-08	1.1E-07				6%	-11.8	-11.7	-13.8
VANCOMYCIN		37332-99-3	37332993	6458	PharmaUBA	5799	1449													6%	-11.9	-11.7	-13.5
Triclosan		3380-34-5	3380345	48	Reach_1954	5800	290	136.8	6.2E-04	3.0E+00	4.6E+04	8.8		2.2E-09	1.1E-08	3.5E-08				13%	-11.9	-11.7	-12.8
Sulfapyridine		144-83-2	144832	29	Reach_1196	5801	249	176.4	5.5E-06	2.5E+03	3.4E+00	8.78	11	4.3E-09	1.1E-07	1.1E-06				12%	-11.9	-11.7	-12.7
Chloramphenicol		56-75-7	56757	64	PharmaBeta_407	5802	323	216.4	2.3E-10	3.5E+03	8.3E+00	9.3		1.1E-07	3.5E-08	1.1E-07				7%	-11.7	-11.7	-13.4
Loratadine		79794-75-5	79794755	3783	PharmaBeta_460	5803	383	201.2	1.2E-06	3.4E-02	4.6E+05		9.25	1.1E-06	1.1E-07	3.5E-07				7%	-11.7	-11.7	-14.0
Glibenclamide		10238-21-8	10238218	152	PharmaBeta_301	5804	494	310.2	4.2E-13	4.0E-01	6.2E+04	5.2	15	1.1E-07	1.1E-07	3.5E-07				9%	-11.7	-11.7	-13.5
Chloroquine Phosphate		50-63-5	50635	6280	PharmaBeta_410	5805	516													6%	-12.0	-11.7	-13.5
Montelukast		158966-92-8	158966928	2066	PharmaBeta_517	5806	586	320.7	5.5E-19	2.8E-05	3.3E+09	4.73	10.6	3.5E-07	3.5E-08	1.1E-07				13%	-11.8	-11.8	-12.7
Estradiol		50-28-2	50282	55	Reach_7	5807	272	152.4	2.7E-07	8.8E+00	8.7E+03	10		9.5E-08	3.5E-07	1.1E-06				8%	-11.8	-11.8	-13.5
Oxybutynin		5633-20-5	5633205	3190	PharmaBeta_585	5808	358	185.8	2.3E-08	1.4E+01	9.1E+03	11.5	5.74	1.1E-06	1.1E-07	3.5E-07				3%	-11.7	-11.8	-14.2
Clonazepam		1622-61-3	1622613	500	PharmaBeta_403	5809	316	217.8	9.8E-09	2.1E+01	3.4E+02	10.6	12	5.4E-08	3.5E-08	1.1E-07				9%	-11.9	-11.8	-13.3
Levonorgestrel		79794-75-5	79794755	3782	PharmaBeta_448	5810	312	168.7	1.3E-07	1.4E+00	3.0E+03	13.6		1.1E-06	1.1E-07	3.5E-07				2%	-11.8	-11.8	-14.3
Tinidazole		193-91-8	193918	-	-	5811														6%	-12.0	-11.8	-13.6
Digoxin		2098-66-0	2098660	529	PharmaBeta_169	5812	781	349.8	4.4E-28	6.9E-02	3.2E+00	13.3		1.6E-07	1.1E-07	3.5E-07				6%	-11.8	-11.8	-13.7
Tolfenamic Acid		13710-19-5	13710195	1177	PharmaUBA	5813	262	159.9	9.8E-06	5.8E+00	2.4E+05	4.22		1.3E-08	1.1E-07	3.5E-07				12%	-11.6	-11.8	-13.3
CEFUROXIME		55268-75-2	55268752	3165	PharmaBeta_123	5814	424	289.4	2.3E-13	6.9E+03	1.9E+00	2.86		1.1E-06	1.1E-07	3.5E-07				1%	-11.4	-11.8	-14.4
Chlorothiazide		58-94-6	58946	5255	PharmaUBA	5815	296	229.5	8.5E-11	5.0E+02	5.9E-01	6.7		3.5E-07	1.1E-07	3.5E-07				3%	-11.7	-11.8	-14.0
Nystatin		1400-61-9	1400619	1925	PharmaBeta_567	5816	276	131.8	1.2E-04	7.0E-01	1.2E+07	4.9		1.1E-06	1.1E-07	3.5E-07				10%	-11.5	-11.8	-13.7
Nicotinamide		98-92-0	98920	1079	Reach_524	5817	122	99.4	2.6E-02	1.8E+05	3.5E-01	14.8	11	2.3E-07	1.1E-07	3.5E-07				4%	-11.9	-11.9	-13.9

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Lorazepam		846-49-1	846491	103	PharmaBeta_461	5818	321	217.5	4.1E-10	1.5E+01	2.6E+02	11.3	13	2.3E-08	3.5E-09	1.1E-08				11%	-11.9	-11.9	-13.1
Promethazine		60-87-7	60877	5422	PharmaUBA	5819	284	143.6	1.4E-03	7.4E+01	3.1E+04		5.2	1.1E-06	3.5E-07	1.1E-06				4%	-12.0	-11.9	-14.3
Albendazole		54965-21-8	54965218	1121	PharmaUBA	5820	265	192.2	2.0E-07	6.5E+00	1.4E+03	9.97	10	7.5E-09	3.5E-08	1.1E-07				12%	-12.1	-11.9	-13.0
Rufinamide		89365-50-4	89365504	5128	PharmaBeta_673	5821	238	161.2	7.8E-05	1.8E+03	2.9E+01	14.7	13.4	1.1E-06	3.5E-07	1.1E-06				2%	-11.9	-11.9	-14.5
Salbutamol		18559-94-9	18559949	2198	Reach_2465	5822	239	145.8	1.2E-06	1.6E+04	4.4E+00	10.1	5.06	1.1E-06	1.1E-07	3.5E-07				1%	-11.6	-11.9	-14.5
Norethisterone		68-22-4	68224	800	Reach_92	5823	298	161.0	3.1E-07	4.7E+00	9.8E+02	13.6		3.0E-07	3.5E-08	1.1E-07				4%	-12.1	-11.9	-14.1
Piracetam		7491-74-9	7491749	3651	PharmaBeta_612	5824	142	131.7	8.5E-04	9.2E+05	4.0E-02	13.6	15.3	3.5E-06	3.5E-07	1.1E-06				1%	-11.3	-12.0	-14.5
Salicylic Acid		69-72-7	69727	84	Reach_95	5825	138	93.8	4.3E-03	5.1E+03	1.7E+02	3		1.6E-06	3.5E-07	1.1E-06				1%	-12.0	-12.0	-14.5
Glipizide		29094-61-9	29094619	4968	PharmaBeta_303	5826	446	300.9	3.6E-14	2.2E+01	2.2E+03	5.2	13.5	1.1E-06	1.1E-07	3.5E-07				2%	-11.9	-12.0	-14.5
Propylthiouracil		51-52-5	51525	5108	PharmaBeta_637	5827	170	164.8	9.2E-06	9.6E+02	9.5E+00	7.5		1.1E-06	3.5E-07	1.1E-06				1%	-11.9	-12.0	-14.5
Meprobamate		57-53-4	57534	5358	PharmaUBA	5828	218	46.6	1.1E-01	9.6E+03	9.5E+00	11.7		1.1E-06	3.5E-07	1.1E-06				1%	-12.2	-12.0	-14.5
Lofepramine		23047-25-8	23047258	5348	PharmaUBA	5829	419	221.6	2.0E-07	4.8E-03	1.8E+07		6.69	1.1E-06	3.5E-07	1.1E-06				10%	-11.6	-12.0	-13.7
Sevelamer		19767-45-4	19767454	5019	PharmaBeta_485	5830	141	72.0	1.0E-02	1.1E+05	1.1E-02	1.21		1.1E-05	1.1E-06	3.5E-06				0%	-11.2	-12.1	-14.3
Imiquimod		26807-65-8	26807658	5331	PharmaUBA	5831	240	190.5	1.0E-06	1.2E+01	1.1E+03		6.7	3.5E-07	3.5E-08	1.1E-07				4%	-12.2	-12.1	-14.2
Cefradine		38821-53-3	38821533	5252	PharmaUBA	5832	349	326.2	9.8E-11	2.8E+03	9.8E-01	2.76	5.61	3.5E-06	3.5E-07	1.1E-06				1%	-11.4	-12.1	-14.6
Ketamine		6740-88-1	6740881	3490	PharmaBeta_381	5833	238	109.6	6.9E-03	1.6E+03	1.3E+03		6.86	3.5E-07	3.5E-08	1.1E-07				4%	-12.3	-12.1	-14.2
Meropenem		119478-56-7	119478567	5622	PharmaBeta_483	5834	438													6%	-12.3	-12.1	-13.9
Ephedrine Hydrochloride		50-98-6	50986	5902	Reach_11	5835	202													6%	-12.3	-12.1	-13.9
Dapsone		80-08-0	80080	3787	Reach_256	5836	248	182.9	3.6E-06	2.1E+03	5.9E+00		12.2	1.1E-06	3.5E-07	1.1E-06				1%	-12.0	-12.1	-14.6
Perindopril		82834-16-0	82834160	5090	PharmaBeta_604	5837	368	309.8	7.5E-10	8.3E+00	3.9E+02	3.07	8.28	3.5E-06	3.5E-07	1.1E-06				1%	-11.8	-12.1	-14.6
Sulfinpyrazone		15676-16-1	15676161	5453	PharmaUBA	5838	404	275.2	9.6E-11	5.9E-02	1.4E+02	3		1.1E-06	1.1E-07	3.5E-07				2%	-12.0	-12.1	-14.6
Ribavirin		36791-04-5	36791045	2778	PharmaBeta_654	5839	244	207.5	6.8E-11	3.0E+05	9.3E-03	14.2	13.9	3.5E-06	3.5E-07	1.1E-06				1%	-11.3	-12.1	-14.6
Eprosartan		133040-01-4	133040014	1864	PharmaBeta_210	5840	425	285.2	4.5E-13	3.4E-01	2.3E+06	3.51	6.91	3.5E-06	3.5E-07	1.1E-06				8%	-11.9	-12.1	-14.1
Vardenafil		224785-90-4	224785904	2334	Reach_4232	5841	489	342.0	4.6E-17	2.9E+01	6.2E+02		5.93	3.5E-07	1.1E-07	3.5E-07				4%	-12.2	-12.1	-14.3
Exemestane		104227-87-4	104227874	5306	PharmaUBA	5842	296	155.1	1.5E-04	4.8E+01	8.9E+02			1.1E-06	1.1E-07	3.5E-07				2%	-12.3	-12.1	-14.6
Doxepin		469-21-6	469216	5291	PharmaUBA	5843	279	133.3	2.6E-03	6.2E+00	9.8E+03		5.2	1.1E-06	1.1E-07	3.5E-07				3%	-12.4	-12.1	-14.6
Haloperidol		52-86-8	52868	3079	PharmaBeta_313	5844	376	194.2	2.0E-08	9.4E+00	1.6E+04	13.7	5.32	3.5E-08	1.1E-08	3.5E-08				10%	-12.3	-12.1	-13.5
Nateglinide		105816-04-4	105816044	5060	PharmaBeta_531	5845	317	209.0	6.4E-08	2.3E-01	5.0E+04	3.29		1.1E-06	1.1E-07	3.5E-07				4%	-12.1	-12.2	-14.6
Tadalafil		209860-87-7	209860877	5139	PharmaBeta_710	5846	389	273.4	2.9E-12	4.3E+00	2.6E+01	15.7	15.8	1.1E-06	1.1E-07	3.5E-07				2%	-11.9	-12.2	-14.7
Acipimox		578-95-0	578950	5216	PharmaUBA	5847	154	135.2	6.2E-04	7.6E+04	3.0E-01	3.3		1.1E-06	1.1E-07	3.5E-07				1%	-11.8	-12.2	-14.7
Fusidic Acid		6990-06-3	6990063	5322	PharmaUBA	5848	517	264.9	3.4E-14	1.0E-01	5.6E+06	4.07		1.1E-06	1.1E-07	3.5E-07				9%	-11.9	-12.2	-14.1
LEVOMEPROMAZINE		60-99-1	60991	3322	PharmaBeta_447	5849	328	171.6	1.2E-05	7.4E+00	1.1E+05		4.81	1.1E-06	1.1E-07	3.5E-07				5%	-12.2	-12.2	-14.6
Teicoplanin		108736-35-2	108736352	6461	PharmaUBA	5850	1804													6%	-12.4	-12.2	-14.0
Tiaprofenic Acid		33005-95-7	33005957	5463	PharmaUBA	5851	260	163.4	1.3E-04	1.3E+01	6.6E+02	3.77		1.1E-06	1.1E-07	3.5E-07				2%	-12.5	-12.2	-14.7
Dexibuprofen		24584-09-6	24584096	4891	PharmaBeta_163	5852	206	94.2	2.5E-02	2.8E+01	6.2E+03	4.3		1.1E-06	1.1E-07	3.5E-07				3%	-12.5	-12.2	-14.7
Lormetazepam		1977-10-2	1977102	5350	PharmaUBA	5853	335	207.6	6.4E-10	1.0E+01	1.7E+02	13.6	13	1.1E-08	3.5E-09	1.1E-08				12%	-12.3	-12.2	-13.4
Piroxicam		33817-20-8	33817208	5417	PharmaUBA	5854	331	245.9	2.3E-12	1.3E+01	3.8E+02	5.5	11.6	3.5E-06	3.5E-07	1.1E-06				1%	-12.0	-12.3	-14.7
VILDAGLIPTIN		274901-16-5	274901165	2510	PharmaBeta_786	5855	303	190.3	1.3E-08	1.1E+02	6.2E+00	15.4	6.41	1.1E-06	1.1E-07	3.5E-07				1%	-11.9	-12.3	-14.8
Mupirocin		126544-47-6	126544476	1806	PharmaBeta_522	5856	501	273.2	2.1E-16	4.8E+00	9.1E+02	4.9		1.1E-06	1.1E-07	3.5E-07				2%	-12.2	-12.3	-14.8
Midazolam		59467-70-8	59467708	736	PharmaBeta_502	5857	326	200.7	6.8E-07	6.7E+01	2.1E+04		8	3.4E-08	1.1E-08	1.1E-08				11%	-12.4	-12.3	-13.7
Isosorbide Dinitrate		87-33-2	87332	3926	Reach_308	5858	236	82.1	8.0E-02	4.5E+04	5.8E+00			1.1E-06	1.1E-07	3.5E-07				1%	-12.2	-12.3	-14.8
Dasatinib		201530-41-8	201530418	4888	PharmaBeta_151	5859	488	304.6	1.2E-17	4.4E-01	1.3E+01	13.6	6.29	3.5E-07	3.5E-08	3.5E-07				3%	-12.3	-12.3	-14.5
Ivabradine		78649-41-9	78649419	4986	PharmaBeta_352	5860	469	251.9	8.7E-11	3.5E-01	5.0E+03		5.62	1.1E-06	3.5E-08	1.1E-07				3%	-12.3	-12.4	-14.9
Megestrol Acetate		3562-63-8	3562638	5355	PharmaUBA	5861	342	182.9	4.6E-08	4.7E+01	2.6E+03	13.9		1.1E-06	1.1E-07	3.5E-07				2%	-12.4	-12.4	-14.9
Colchicine		64-86-8	64868	782	Reach_75	5862	399	241.8	4.2E-09	1.4E+01	7.2E+01	14.6	15	2.1E-07	1.1E-07	3.5E-07				5%	-12.5	-12.4	-14.4
Deferasirox		30652-11-0	30652110	4889	PharmaBeta_153	5863	373	272.3	2.2E-14	1.5E+00	2.8E+03	5.58	13.8	3.5E-07	3.5E-08	1.1E-07				4%	-12.5	-12.4	-14.6
Cefaclor		5575-21-3	5575213	5241	PharmaUBA	5864	368	327.7	3.0E-13	3.0E+03	2.2E+00	1.64	6.66	3.5E-06	3.5E-07	1.1E-06				1%	-11.8	-12.4	-14.9
Dexpanthenol		81-13-0	81130	3802	Reach_272	5865	205	161.4	2.0E-06	1.3E+05	1.2E-02	13.2	15.5	1.1E-06	3.5E-07	1.1E-06				1%	-12.0	-12.4	-14.9
IMATINIB		152459-95-5	152459955	2024	PharmaBeta_332	5866	494	313.4	4.8E-15	5.1E-01	1.0E+03	15	6.43	1.1E-06	3.5E-07	1.1E-06				2%	-12.4	-12.4	-14.9
Nebivolol		99200-09-6	99200096	5062	PharmaBeta_542	5867	405	214.5	5.7E-11	6.3E+00	5.1E+03	13.5	5.81	1.1E-06	3.5E-08	1.1E-07				3%	-12.4	-12.4	-14.9
Almotriptan		177036-94-1	177036941	4835	PharmaBeta_25	5868	335	207.1	8.5E-08	9.7E+02	1.3E+02	15.7	5.36	3.5E-07	3.5E-08	1.1E-07				4%	-12.4	-12.5	-14.6
CINACALCET		226256-56-0	226256560	4876	PharmaBeta_132	5869	357	151.9	2.1E-05	5.7E-01	6.0E+06		4.54	3.5E-07	1.1E-08	3.5E-08				10%	-12.4	-12.5	-14.4
Fenoprofen		13392-18-2	13392182	5310	PharmaUBA	5870	242	136.5	3.1E-03	2.2E+01	7.9E+03	4.27		1.1E-06	1.1E-07	3.5E-07				3%	-12.8	-12.5	-15.0
Zolmitriptan		139264-17-8	139264178	1918	PharmaBeta_800	5871	287	201.7	1.9E-07	1.5E+03	8.3E+01	12	5.3	3.5E-07	3.5E-08	1.1E-07				3%	-12.4	-12.5	-14.7
MECLOZINE		569-65-3	569653	3218	PharmaBeta_476	5872	391	204.8	1.2E-01	4.5E-01	7.4E+05		8.12	3.5E-07	1.1E-07	1.1E-07				10%	-12.7	-12.5	-14.4
FLUPENTIXOL		2709-56-0	2709560	2495	PharmaBeta_269	5873	435	215.9	1.4E-10	5.6E-01	1.2E+04	14.9	6.29	1.1E-07	1.1E-08	3.5E-08				8%	-12.7	-12.6	-14.3
Torasemide		56211-40-6	56211406	5165	PharmaBeta_754	5874	348	225.3	5.3E-09	1.0E+01	8.9E+01	6.65		3.5E-07	1.1E-07	3.5E-07				3%	-12.7	-12.6	-14.8
Moxifloxacin		354812-41-2	354812412	2017	PharmaBeta_519	5875	401	325.0	9.7E-13	1.3E+02	8.9E+00	6.11	5.28	1.1E-06	1.1E-07	3.5E-07				1%	-12.3	-12.6	-15.2
DESMOPRESSIN		16679-58-6	16679586	6397	PharmaBeta_159	5876	1069													6%	-12.9	-12.7	-14.5
Rizatriptan		162401-32-3	162401323	5123	PharmaBeta_664	5877	269	177.2	7.4E-06	1.5E+02	2.8E+01		5.3	1.1E-06	3.5E-08	1.1E-07				2%	-12.4	-12.7	-15.2
Tacrolimus		104987-11-3	104987113	5455	PharmaUBA	5878	804	349.8	1.1E-29	3.4E-03	1.1E+03	10.1		1.1E-06	1.1E-07	3.5E-07				2%	-13.0	-12.7	-15.2
Famciclovir		58306-30-2	58306302	5307	PharmaUBA	5879	321	202.0	1.5E-07	3.0E+02	4.4E+00		10.1	3.5E-06	3.5E-07	1.1E-06				1%	-12.2	-12.7	-15.3
GOSERELIN		65807-02-5	65807025	6403	PharmaBeta_309	5880	1270													6%	-13.0	-12.7	-14.5
Saxagliptin		28523-86-6	28523866	5131	PharmaBeta_680	5881	315	195.1	5.6E-09	9.5E+01	9.5E+00	15.6	6.58	1.1E-06	1.1E-07	3.5E-07				1%	-12.4	-12.7	-15.3
Lamivudine		134678-17-4	134678174	1881	PharmaBeta_427	5882	229	164.5	1.1E-06	1.7E+03	2.4E-03	14.1	9.75	3.5E-06	1.1E-06	3.5E-06				1%	-12.2	-12.8	-15.3
Nalidixic Acid		389-08-2	389082	5376	PharmaUBA	5883	232	164.6	8.2E-06	6.5E+01	4.4E+01	6.22	9.5	1.1E-06	3.5E-07	1.1E-06				2%	-12.8	-12.8	-15.3
Capsaicin		404-86-4	404864	627	PharmaBeta_114	5884	305	196.5	1.8E-06	4.8E+00	1.0E+04	10	14	3.1E-07	1.1E-07	3.5E-07				5%	-12.9	-12.8	-14.9
Tibolone		5630-53-5	5630535	3189	PharmaBeta_735	5885	312	170.7	4.1E-07	1.2E+00	1.8E+03	13.6		3.5E-07	3.5E-08	1.1E-07				4%	-12.9	-12.8	-14.9
Agomelatine		56180-94-0	56180940	4831	PharmaBeta_13	5886	243	168.1	9.7E-06	7.6E+00	5.8E+02	14.8	14.5	1.1E-06	3.5E-08	1.1E-07				2%	-12.8	-12.8	-15.3
Retigabine		155213-67-5	155213675	5121	PharmaBeta_653	5887	303	172.1	7.5E-06	9.1E+00	3.6E+02	13.2	8.94	1.1E-06	1.1E-07	1.1E-06				2%	-12.9	-12.8	-15.3
Prasterone		53-43-0	53430	3101	Reach_20	5888	288	144.6	3.3E-06	3.6E+01	9.5E+02	16		3.5E-07	3.5E-08	1.1E-07				4%	-12.9	-12.8	-15.0
TERAZOSIN		63590-64-7	63590647	3413	PharmaBeta_725	5889	387	239.8	2.2E-10	4.4E+02	3.0E+01		6.57	1.1E-06	1.1E-07	3.5E-07				2%	-12.6	-12.8	-15.3
Pindolol		137-58-6	137586	23	PharmaBeta_609	5890	248	145.8	8.5E-07	6.7E+03	3.0E+01	14.1	4.5	1.8E-07	1.1E-07	3.5E-07				5%	-12.9	-12.8	-14.8
Praziquantel		31218-83-4	31218834	1159	PharmaUBA	5891	312	202.4	9.9E-07	1.6E+02	2.6E+02		16	5.9E-08	1.1E-07	3.5E-07				9%	-13.1	-12.9	-14.4
TAPENTADOL		175591-23-8	175591238	5142	PharmaBeta_715	5892	221	82.3	1.6E-02	3.1E+02	3.7E+03	10.2	4.82	1.1E-06	1.1E-07	3.5E-07				2%	-13.1	-12.9	-15.4

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Dutasteride		496775-61-2	496775612	4918	PharmaBeta_194	5893	529	262.4	1.7E-11	1.1E-02	9.8E+04	13	14.6	3.5E-07	1.1E-07	3.5E-07				7%	-12.8	-12.9	-15.0
Tetrabenazine		58-46-8	58468	5154	PharmaBeta_730	5894	317	157.8	7.1E-05	1.7E+01	4.6E+02		7.02	1.1E-06	1.1E-07	3.5E-07				2%	-13.1	-12.9	-15.4
Desogestrel		54024-22-5	54024225	3117	PharmaBeta_160	5895	310	148.8	8.3E-06	3.8E-02	4.5E+05	13.6		3.5E-07	3.5E-08	1.1E-07				8%	-13.0	-12.9	-15.0
Perphenazine		58-39-9	58399	3246	PharmaBeta_603	5896	404	223.2	1.0E-09	5.7E+00	6.6E+03	14.9	6.13	1.1E-06	3.5E-08	1.1E-07				3%	-12.9	-12.9	-15.4
Caffeine		58-08-2	58082	66	Reach_45	5897	194	180.3	9.8E-07	3.2E+05	1.4E+00			6.8E-09	1.1E-07	3.5E-07				12%	-13.1	-12.9	-14.1
Diethylstilbestrol		128-46-1	128461	1133	PharmaUBA	5898	268	151.8	1.2E-06	8.9E-01	4.4E+05	9.7		9.6E-09	3.5E-08	1.1E-07				12%	-12.8	-13.0	-14.4
Rotigotine		106308-44-5	106308445	5127	PharmaBeta_671	5899	315	176.9	9.9E-07	3.3E+01	2.5E+05	10.2	5.44	3.5E-07	3.5E-08	1.1E-07				8%	-13.0	-13.0	-15.1
Lanreotide		129805-33-0	129805330	6462	PharmaBeta_429	5900	1037													6%	-13.2	-13.0	-14.8
Piperazine		110-85-0	110850	1531	Reach_832	5901	86	7.3	9.5E+01	1.0E+06	1.6E-01		4.4	3.5E-06	3.5E-07	1.1E-06				1%	-13.2	-13.0	-15.5
Mesterolone		1424-00-6	1424006	1955	Reach_1679	5902	304	144.5	4.6E-07	4.0E+00	3.0E+03	16		3.5E-07	3.5E-08	1.1E-07				4%	-13.2	-13.0	-15.2
Triptorelin		7722-84-1	7722841	6451	PharmaBeta_766	5903	1241													6%	-13.3	-13.0	-14.8
Buprenorphine		52485-79-7	52485797	3061	PharmaBeta_107	5904	468	226.0	2.3E-11	1.2E-01	7.9E+04	9.77	5.74	1.1E-06	1.1E-07	3.5E-07				5%	-13.1	-13.2	-15.6
Estriol		50-27-1	50271	54	PharmaBeta_225	5905	288	180.7	1.2E-09	5.1E+01	6.5E+02	10		1.0E-07	1.1E-07	3.5E-07				7%	-13.3	-13.2	-14.9
Prasugrel		81093-37-0	81093370	5100	PharmaBeta_622	5906	373	190.9	9.8E-07	4.0E+01	8.3E+03		8.03	1.1E-06	1.1E-07	3.5E-07				3%	-13.2	-13.2	-15.7
Minoxidil		38304-91-5	38304915	2820	PharmaBeta_508	5907	209	173.1	1.8E-06	2.8E+04	2.2E+01		9.4	1.1E-06	3.5E-08	1.1E-07				2%	-12.8	-13.2	-15.7
Triamcinolone Acetonide		76-25-5	76255	5469	PharmaUBA	5908	435	223.4	1.5E-12	4.4E+01	4.9E+02	13.2		1.1E-06	1.1E-07	3.5E-07				2%	-13.2	-13.2	-15.7
Eletriptan		143322-58-1	143322581	1963	PharmaBeta_199	5909	383	234.2	1.4E-09	1.2E+01	3.2E+03		4.83	1.1E-06	3.5E-08	1.1E-07				2%	-13.2	-13.3	-15.8
Zidovudine		30516-87-1	30516871	2602	PharmaBeta_796	5910	267	308.1	1.2E-15	2.6E+03	1.7E+00	9.6		3.5E-06	3.5E-07	1.1E-06				1%	-12.7	-13.3	-15.8
Phenylephrine Hydrochloride		61-76-7	61767	5952	Reach_60	5911	204													6%	-13.5	-13.3	-15.1
Tenoxicam		59804-37-4	59804374	5459	PharmaUBA	5912	337	248.6	1.1E-12	6.8E+01	2.5E+02	5.5	13	1.1E-06	1.1E-07	3.5E-07				2%	-13.2	-13.3	-15.8
Guaifenesin		93-14-1	93141	4061	PharmaBeta_312	5913	198	100.0	3.4E-04	1.2E+05	2.6E+00	14		1.1E-06	1.1E-07	3.5E-07				1%	-13.0	-13.3	-15.8
Melatonin		73-31-4	73314	3619	PharmaBeta_477	5914	232	182.5	1.8E-05	8.8E+02	4.5E+01	15.1	14.3	1.1E-06	1.1E-07	3.5E-07				2%	-13.2	-13.3	-15.9
Pimecrolimus		111025-46-8	111025468	5096	PharmaBeta_608	5915	810	349.8	1.1E-27	5.1E-04	2.5E+04	10.1		1.1E-06	1.1E-07	3.5E-07				4%	-13.6	-13.3	-15.8
Rifaximin		19395-41-6	19395416	5429	PharmaUBA	5916	787	349.8	4.6E-33	6.7E-06	6.5E+07	4.15	11.5	3.5E-07	1.1E-07	3.5E-07				12%	-12.8	-13.3	-14.7
Atazanavir		198904-31-3	198904313	2244	PharmaBeta_57	5917	705	349.8	1.4E-24	1.1E-02	7.6E+02	8.78	10.1	3.5E-07	1.1E-07	3.5E-07				4%	-13.5	-13.4	-15.5
Acitretin		55079-83-9	55079839	3159	PharmaBeta_9	5918	326	172.8	4.0E-07	1.5E-01	1.5E+07	4.4		3.5E-07	3.5E-08	3.5E-07				11%	-13.0	-13.4	-15.0
Etonogestrel		54048-10-1	54048101	3119	PharmaBeta_229	5919	324	175.5	1.7E-07	4.9E-01	7.8E+03	13.6		3.5E-07	3.5E-08	1.1E-07				5%	-13.5	-13.4	-15.5
Pyrimethamine		58-14-0	58140	1161	PharmaUBA	5920	249	176.5	1.8E-06	7.4E+01	2.6E+02		7	4.1E-09	1.1E-07	3.5E-07				12%	-13.6	-13.4	-14.5
Deferiprone		51146-56-6	51146566	4890	PharmaBeta_154	5921	139	71.9	2.1E-02	2.1E+04	4.5E-01	8.7	11.6	3.5E-06	3.5E-07	1.1E-06				1%	-13.0	-13.4	-16.0
Acrivastine		87848-99-5	87848995	5218	PharmaUBA	5922	348	318.1	2.1E-11	5.3E+00	1.2E+02	4.26	4.51	3.5E-06	3.5E-07	1.1E-06				1%	-13.1	-13.5	-15.9
Alfentanil		71195-58-9	71195589	3578	PharmaBeta_19	5923	417	239.4	8.5E-09	2.7E+02	2.3E+02		7.47	3.5E-07	3.5E-08	1.1E-07				4%	-13.5	-13.5	-15.6
Glimepiride		93479-97-1	93479971	4070	PharmaBeta_302	5924	491	329.6	3.5E-16	4.0E+00	5.0E+04	5.17	14.1	1.1E-06	1.1E-07	3.5E-07				4%	-13.4	-13.5	-15.9
Probenecid		57-66-9	57669	3237	PharmaBeta_628	5925	285	179.9	3.0E-06	2.5E+03	7.8E+02	3.6		3.5E-06	3.5E-07	1.1E-06				1%	-13.3	-13.5	-16.0
Darunavir		302962-49-8	302962498	4887	PharmaBeta_150	5926	548	296.5	5.4E-17	9.2E-02	7.6E+01	9.94	12.2	1.1E-06	1.1E-07	3.5E-07				2%	-13.4	-13.5	-16.0
Benzyl Benzoate		120-51-4	120514	359	Reach_996	5927	212	70.8	7.4E-02	7.3E+01	3.5E+03			5.8E-07	1.1E-07	3.5E-07				3%	-13.9	-13.6	-15.8
Isotretinoin		154-21-2	154212	1146	PharmaUBA	5928	300	148.0	1.4E-05	2.8E-01	7.1E+07	4.4		3.6E-08	3.5E-07	1.1E-06				13%	-12.9	-13.6	-14.9
Nimodipine		104206-65-7	104206657	5068	PharmaBeta_554	5929	418	208.6	6.8E-08	1.2E+00	1.3E+03		12.2	1.1E-06	1.1E-07	3.5E-07				2%	-13.7	-13.6	-16.1
Efavirenz		154598-52-4	154598524	2038	PharmaBeta_196	5930	316	164.2	5.0E-05	3.2E+00	4.9E+04	11.8		3.5E-07	1.1E-07	3.5E-07				6%	-13.8	-13.7	-15.8
Betaxolol		63659-18-7	63659187	4850	PharmaBeta_87	5931	307	140.7	9.8E-06	7.0E+02	9.5E+02	13.9	4.5	1.1E-06	1.1E-07	3.5E-07				2%	-13.7	-13.7	-16.2
Repaglinide		135062-02-1	135062021	1886	PharmaBeta_651	5932	453	274.2	2.6E-12	5.9E-02	1.5E+06	3.61	8.05	1.1E-06	1.1E-07	3.5E-07				8%	-13.6	-13.8	-15.9
Cefpodoxime		82619-04-3	82619043	5250	PharmaUBA	5933	427	303.0	2.6E-14	1.8E+03	8.1E-01	2.26	10.4	1.1E-06	1.1E-07	1.1E-06				1%	-13.5	-13.8	-16.3
Glucagon		76712-82-8	76712828	6429	PharmaBeta_304	5934	3483													6%	-14.0	-13.8	-15.6
Benzoic Acid		65-85-0	65850	785	Reach_77	5935	122	48.9	4.0E-01	3.5E+03	7.4E+01	4.1		1.1E-06	3.5E-07	1.1E-06				2%	-14.1	-13.8	-16.3
Bromocriptine		25614-03-3	25614033	5232	PharmaUBA	5936	655	349.8	8.7E-24	6.8E-03	1.1E+04	9.5	8.82	1.1E-06	1.1E-07	3.5E-07				3%	-13.8	-13.8	-16.3
Cilazapril		88768-40-5	88768405	5515	PharmaUBA	5937	418	323.3	2.1E-12	7.9E+00	1.9E+02	2.99	8.47	1.1E-06	1.1E-07	3.5E-07				2%	-13.8	-13.9	-16.4
Fluticasone		90566-53-3	90566533	4002	PharmaBeta_271	5938	445	211.5	9.9E-11	4.6E+00	2.5E+01	13.2		1.1E-06	3.5E-07	1.1E-06				2%	-13.8	-13.9	-16.4
Diflunisal		125-28-0	125280	5282	PharmaUBA	5939	250	159.8	3.1E-06	6.6E+01	2.6E+04	2.77		1.1E-06	1.1E-07	3.5E-07				4%	-14.0	-14.0	-16.5
Rifabutin		72559-06-9	72559069	3606	PharmaBeta_655	5940	847	349.8	1.2E-31	1.1E-04	3.2E+07	7.16	4.36	1.1E-06	1.1E-07	3.5E-07				10%	-13.7	-14.1	-15.7
Fenbufen		31879-05-7	31879057	5309	PharmaUBA	5941	254	162.0	5.8E-06	1.1E+01	1.5E+03	4.8		3.5E-07	3.5E-08	3.5E-08				4%	-14.2	-14.1	-16.3
Degarelix		214766-78-6	214766786	6424	PharmaBeta_156	5942	1632													6%	-14.3	-14.1	-15.9
Hyoscine		51-34-3	51343	3036	Reach_15	5943	303	151.3	2.6E-07	7.5E+03	2.5E+00	14.1	6.23	1.1E-06	1.1E-07	3.5E-07				1%	-13.7	-14.1	-16.6
Pirenzepine		79548-73-5	79548735	5415	PharmaUBA	5944	351	244.7	2.7E-10	8.2E-02	4.8E+01	14.6	5.9	1.1E-06	3.5E-07	1.1E-06				2%	-14.1	-14.2	-16.7
Isradipine		155974-00-8	155974008	4985	PharmaBeta_350	5945	371	194.9	5.4E-07	3.3E-01	3.1E+03		12	1.1E-06	1.1E-07	3.5E-07				2%	-14.3	-14.2	-16.7
Thalidomide		175591-23-8	175591238	5141	PharmaBeta_713	5946	258	274.7	2.7E-12	2.2E+01	5.8E-01	8.17	14.4	1.1E-06	1.1E-07	3.5E-07				1%	-13.7	-14.2	-16.7
Fentanyl		437-38-7	437387	2914	PharmaBeta_247	5947	336	186.7	8.7E-06	1.8E+02	7.8E+03		5.92	1.1E-06	1.1E-07	3.5E-07				3%	-14.3	-14.3	-16.8
Metolazone		13265-10-6	13265106	5033	PharmaBeta_490	5948	366	237.6	4.7E-10	2.0E+00	6.9E+01	9.69	14.1	3.5E-06	1.1E-07	3.5E-07				1%	-13.9	-14.4	-16.9
Sirolimus		53123-88-9	53123889	3089	PharmaBeta_690	5949	914	349.8	4.1E-34	4.2E-05	6.5E+04	10.4		1.1E-06	1.1E-07	3.5E-07				5%	-14.6	-14.4	-16.8
Bimatoprost		155206-00-1	155206001	4852	PharmaBeta_93	5950	416	267.0	7.0E-16	1.6E+00	9.3E+03	14.7	14.3	1.1E-06	1.1E-07	3.5E-07				3%	-14.4	-14.4	-16.9
Fluocortolone		152-97-6	152976	2026	Reach_1209	5951	376	204.9	5.2E-10	5.4E+01	1.1E+02	13.8		1.1E-06	3.5E-07	1.1E-06				2%	-14.4	-14.4	-16.9
KETOTIFEN		10596-23-3	10596233	4991	PharmaBeta_386	5952	309	184.8	2.4E-06	8.8E+00	7.1E+03		5.4	1.1E-06	1.1E-07	3.5E-07				3%	-14.5	-14.5	-17.0
Thioridazine		55297-95-5	55297955	5460	PharmaUBA	5953	371	201.8	4.9E-06	2.6E-01	2.8E+06		4.61	1.1E-06	3.5E-07	1.1E-06				9%	-14.2	-14.5	-16.5
Raltegravir		132875-61-7	132875617	5118	PharmaBeta_645	5954	444	332.3	6.1E-20	6.7E+01	2.5E+00	8.4	14.7	1.1E-06	1.1E-07	3.5E-07				1%	-14.2	-14.6	-17.1
Tocofersolan		9002-96-4	9002964	5162	PharmaBeta_748	5955	575	253.0	1.1E-13	5.6E-06	2.0E+11	14.2		1.1E-06	1.1E-07	3.5E-07				13%	-14.8	-14.6	-15.4
Acetic Acid		64-19-7	64197	778	Reach_72	5956	60	-21.3	2.3E+03	9.6E+05	1.2E+00	4.9		4.7E-06	3.5E-07	3.5E-07				1%	-15.0	-14.8	-17.1
Phenol		108-95-2	108952	252	Reach_765	5957	94	-2.3	4.3E+01	3.5E+04	3.2E+01	10		9.3E-07	3.5E-07	1.1E-06				2%	-15.3	-15.0	-17.4
Latanoprost		191732-72-6	191732726	5004	PharmaBeta_434	5958	433	229.6	4.3E-13	4.8E+00	4.7E+05	15.2		1.1E-06	1.1E-07	3.5E-07				7%	-14.9	-15.1	-17.3
Fulvestrant		129453-61-8	129453618	414	PharmaBeta_283	5959	607	270.1	1.7E-15	7.0E-07	2.6E+11	10		4.8E-08	1.1E-07	3.5E-07				13%	-15.3	-15.1	-15.9
Benperidol		983-42-6	983426	5506	PharmaUBA	5960	381	227.9	1.7E-08	2.3E+00	3.5E+03	11.5	5.99	1.1E-06	1.1E-07	3.5E-07				2%	-15.1	-15.1	-17.6
Prednisone		53-03-2	53032	5102	PharmaBeta_625	5961	358	213.6	5.1E-11	5.6E+02	3.9E+01	13		1.1E-06	3.5E-07	1.1E-06				2%	-15.1	-15.1	-17.6
Misoprostol		59122-46-2	59122462	3267	PharmaBeta_510	5962	383	192.5	6.1E-10	1.6E+01	3.0E+04	15.1		1.1E-06	1.1E-07	3.5E-07				4%	-15.1	-15.2	-17.6
Tretinoin		57-91-0	57910	1117	PharmaBeta_760	5963	300	148.0	1.4E-05	2.8E-01	7.1E+07	4.4		3.6E-08	3.5E-07	1.1E-06				13%	-14.6	-15.2	-16.5
Alprostadil		745-65-3	745653	3640	PharmaBeta_27	5964	354	217.9	3.1E-11	3.1E+00	5.4E+03	4.9		1.1E-06	1.1E-07	3.5E-07				3%	-15.2	-15.3	-17.7
Salmeterol		62989-33-7	62989337	5129	PharmaBeta_678	5965	416	243.5	2.6E-13	4.4E+01	1.4E+04	10	5.34	1.1E-06	1.1E-07	3.5E-07				3%	-15.3	-15.4	-17.8
Penciclovir		97825-25-7	97825257	5552	PharmaUBA	5966	253	255.8	2.6E-14	2.1E+05	1.4E-02	9.37	10.9	3.5E-06	1.1E-06	3.5E-06				1%	-14.8	-15.4	-18.0
Fluocinonide		356-12-7	356127	5317	PharmaUBA	5967	495	225.2	2.4E-12	4.2E+01	5.9E+02	13.7		3.5E-06	3.5E-07	1.1E-06				1%	-15.3	-15.5	-18.0

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Erlotinib		183321-74-6	183321746	2183	PharmaBeta_216	5968	393	221.6	9.4E-09	1.2E+00	6.2E+02		8.12	1.1E-06	1.1E-07	3.5E-07				2%	-15.5	-15.5	-18.1
Mesna		19767-45-4	19767454	5019	PharmaBeta_485	5969	141	72.0	1.0E-02	1.1E+05	1.1E-02	1.21		1.1E-05	1.1E-06	3.5E-06				0%	-14.7	-15.6	-17.8
Paliperidone		58-74-2	58742	5083	PharmaBeta_588	5970	427	252.9	1.7E-13	3.9E+00	8.9E+01	15.9	5.85	3.5E-06	3.5E-07	1.1E-06				1%	-15.3	-15.6	-18.1
Roflumilast		91374-21-9	91374219	5124	PharmaBeta_665	5971	403	212.9	3.5E-08	3.7E-01	3.4E+03		13	1.1E-06	1.1E-07	3.5E-07				2%	-15.8	-15.8	-18.3
Flunisolide		3385-03-3	3385033	5315	PharmaUBA	5972	435	224.7	8.7E-12	3.0E+01	4.6E+02	13.3		1.1E-06	1.1E-07	3.5E-07				2%	-15.7	-15.8	-18.3
Phenylbutazone		50-33-9	50339	5412	PharmaUBA	5973	308	212.2	6.4E-07	2.8E+01	3.3E+03	4.3		3.5E-06	1.1E-07	3.5E-07				2%	-15.6	-15.8	-18.3
Nitisinone		58691-88-6	58691886	5069	PharmaBeta_555	5974	329	175.3	9.9E-06	8.8E+01	7.6E+03	2.71		1.1E-06	3.5E-08	1.1E-07				3%	-15.8	-15.9	-18.4
Travoprost		81846-19-7	81846197	5172	PharmaBeta_758	5975	501	238.2	1.9E-13	8.0E-02	2.9E+05	14.1		1.1E-06	1.1E-07	3.5E-07				6%	-15.8	-15.9	-18.2
Busulfan		55-98-1	55981	708	PharmaBeta_110	5976	246	129.8	1.2E-05	1.5E+04	2.1E-01			1.1E-06	3.5E-07	1.1E-06				1%	-15.6	-15.9	-18.5
Aprepitant		170729-80-3	170729803	2120	PharmaBeta_53	5977	534	270.1	4.9E-12	1.9E-02	1.0E+03		10.4	1.1E-06	1.1E-07	3.5E-07				2%	-16.2	-16.2	-18.7
Entecavir		142217-69-4	142217694	4922	PharmaBeta_205	5978	277	265.5	4.0E-15	1.3E+05	6.2E-02	9.34	10.9	3.5E-06	1.1E-06	3.5E-06				1%	-15.8	-16.4	-18.9
Dydrogesterone		152-62-5	152625	5293	PharmaUBA	5979	312	150.6	9.6E-05	3.5E+01	2.8E+03			1.1E-06	1.1E-07	3.5E-07				2%	-16.6	-16.4	-18.9
Ivermectin		16846-24-5	16846245	5343	PharmaUBA	5980	875	349.8	1.6E-28	2.6E-04	4.1E+04	12.8		1.1E-06	1.1E-07	3.5E-07				4%	-16.6	-16.4	-18.9
Everolimus		159351-69-6	159351696	2068	PharmaBeta_235	5981	958	349.8	1.4E-35	2.4E-05	3.4E+04	10.4		1.1E-06	1.1E-07	3.5E-07				4%	-16.7	-16.5	-18.9
Fumaric Acid		110-17-8	110178	276	Reach_807	5982	116	84.1	1.3E-09	5.5E+04	1.1E+00	3		4.7E-06	3.5E-07	1.1E-06				1%	-15.9	-16.6	-19.1
NAFARELIN		83150-76-9	83150769	6440	PharmaBeta_525	5983	1323													6%	-16.9	-16.7	-18.5
Tafluprost		50-35-1	50351	5140	PharmaBeta_711	5984	453	204.6	5.1E-11	1.0E-01	3.2E+06	15.1		1.1E-06	1.1E-07	3.5E-07				9%	-16.4	-16.7	-18.7
Zanamivir		139110-80-8	139110808	1916	PharmaBeta_795	5985	332	268.0	5.8E-16	1.1E+04	2.2E-05	3.46	0.74	3.5E-06	3.5E-07	1.1E-06				1%	-16.0	-16.8	-19.3
Triamcinolone		124-94-7	124947	1795	PharmaBeta_761	5986	394	229.9	3.2E-13	3.4E+02	9.1E+00	12.4		1.1E-06	3.5E-07	1.1E-06				1%	-16.8	-17.0	-19.5
Nepafenac		54-11-5	54115	5066	PharmaBeta_546	5987	254	198.8	3.0E-07	1.2E+02	4.0E+01	15	12.6	1.1E-06	1.1E-07	3.5E-07				2%	-17.0	-17.2	-19.7
Cetrorelix		120287-85-6	120287856	6418	PharmaBeta_126	5988	1431													6%	-17.6	-17.4	-19.2
Flumazenil		78755-81-4	78755814	4957	PharmaBeta_262	5989	303	205.4	1.2E-07	2.6E+01	1.1E+01		12	1.1E-06	1.1E-07	3.5E-07				1%	-17.7	-17.9	-20.4
NANDROLONE		437-38-7	437387	2914	PharmaBeta_247	5990	336	186.7	8.7E-06	1.8E+02	7.8E+03		5.92	1.1E-06	1.1E-07	3.5E-07				3%	-19.2	-19.2	-21.6
Metronidazole		443-48-1	443481	642	PharmaBeta_493	5991	171	127.5	1.7E-05	7.3E+03		15.6	11	8.8E-08	3.5E-08	1.1E-07				0%			
Ciprofloxacin		86386-73-4	86386734	969	PharmaBeta_135	5992	331	316.7	3.8E-11	1.2E+03		5.86	5	6.3E-09	1.1E-07	3.5E-07				0%			
Tobramycin		32986-56-4	32986564	2672	PharmaBeta_747	5993	468	305.7	3.2E-19	1.0E+06	1.7E-06	12.1	5.01	3.5E-06	3.5E-07	1.1E-06				1%			
Amikacin		37517-28-5	37517285	2801	PharmaBeta_36	5994	586	349.8	7.7E-26	1.0E+06	1.7E-09	11.9	4.73	3.5E-06	3.5E-07	1.1E-06				1%			
Tigecycline		69004-04-2	69004042	5559	PharmaUBA	5995	586	349.8	1.2E-27	1.6E+02	6.3E-01	3.15	4.45	3.5E-07	1.1E-07	3.5E-07				3%			
Pesticides																							
count							*409*	*409*	*409*	*409*	*409*	*409*	*409*	*409*	*409*	*409*	*420*	*0*	*420*	*420*	*420*	*420*	*420*
sum																	*1.8E+05*		*1.8E+05*	*100%*			
standard deviation																					*1.2*	*1.2*	*1.2*
2.5-p																	*6.9E-01*		*6.9E-01*	*100%*	*-11.2*	*-11.4*	*-12.9*
50-p																	*5.8E+01*		*5.8E+01*	*100%*	*-8.7*	*-9.0*	*-10.2*
97.5-p																	*2.4E+03*		*2.4E+03*	*100%*	*-6.7*	*-6.8*	*-8.3*
Sulphur		7704-34-9	7704349	6446	Pest_418	5997														100%	-4.9	-4.9	-6.6
Mancozeb		8018-01-7	8018017	1185	Pest_242	5998	541	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				100%	-5.5	-5.5	-7.2
Glyphosate		1071-83-6	1071836	212	Pest_15	5999	169	204.2	1.7E-07	8.7E+03	1.7E-05	0.48	4	5.5E-07	1.1E-07	3.5E-07				100%	-5.1	-5.6	-7.9
Chlormequat		7003-89-6	7003896	4871	Pest_302	6000	123	121.5	1.7E-03	2.2E+05	3.6E-02	0	0	3.5E-07	3.5E-08	1.1E-07				100%	-5.5	-5.9	-8.0
Isoproturon		34123-59-6	34123596	49	Pest_157	6001	206	108.8	1.0E-03	7.7E+01	6.9E+02	14.3	13.9	1.1E-08	3.5E-08	1.1E-07				100%	-6.0	-6.1	-7.1
Metiram		9006-42-2	9006422	6288	Pest_377	6002	276	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				100%	-6.3	-6.2	-8.0
Atrazine		1912-24-9	1912249	37	Reach_1734	6003	216	113.9	3.8E-03	1.5E+01	6.6E+02	0	12.3	2.2E-09	1.1E-07	1.1E-07				100%	-6.5	-6.5	-8.2
Copper oxychloride		1332-40-7	1332407	6252	Pest_310	6004	249	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				100%	-6.5	-6.5	-8.3
Terbuthylazine		5915-41-3	5915413	70	Pest_201	6005	230	123.5	2.1E-03	9.2E-01	1.9E+03	0	12.3	2.5E-09	3.5E-08	1.1E-07				100%	-6.6	-6.6	-8.3
Ziram		137-30-4	137304	6353	Pest_436	6006														100%	-6.8	-6.7	-8.5
Metazachlor		67129-08-2	67129082	81	Pest_215	6007	278	164.1	1.5E-04	8.7E+01	2.4E+02	0	13.6	6.3E-08	3.5E-08	1.1E-07				100%	-6.5	-6.8	-8.2
Chloridazon		1698-60-8	1698608	35	Pest_93	6008	222	154.8	1.5E-04	1.0E+02	5.8E+00	0	10.7	5.2E-08	3.5E-07	1.1E-06				100%	-6.9	-6.8	-8.6
Propineb		12071-83-9	12071839	6443	Pest_402	6009														100%	-6.9	-6.9	-8.6
Copper		7440-50-8	7440508	6419	Pest_305	6010														100%	-7.0	-6.9	-8.7
2,4-D		94-75-7	94757	111	Pest_278	6011	221	109.1	3.7E-03	5.0E+02	4.2E+02	2.97	0	7.5E-08	1.1E-07	3.5E-07				100%	-6.8	-7.0	-8.3
MCPA		94-74-6	94746	110	Pest_369	6012	201	101.0	6.0E-02	8.4E+02	3.3E+02	3.05	0	6.6E-08	1.1E-07	1.1E-06				100%	-7.2	-7.1	-8.2
Dimethomorph		110488-70-5	110488705	4906	Pest_330	6013	388	210.8	2.6E-07	5.4E+00	2.3E+02	0	15.8	1.1E-07	3.5E-08	3.5E-08				100%	-6.7	-7.1	-8.8
Thiram		137-26-8	137268	441	Reach_1137	6014	240	107.3	1.5E-03	3.9E+02	5.0E+01	0	16	2.4E-08	1.1E-07	3.5E-07				100%	-6.9	-7.1	-8.3
Acetochlor		34256-82-1	34256821	608	Pest_158	6015	270	128.5	3.7E-03	8.7E+02	2.3E+03	0	0	5.0E-08	3.5E-08	1.1E-07				100%	-6.9	-7.2	-8.4
Metamitron		41394-05-2	41394052	632	Pest_173	6016	202	157.9	9.9E-05	9.4E+03	2.8E+01	0	11	1.8E-08	3.5E-07	1.1E-06				100%	-7.2	-7.2	-8.9
Copper sulphate		7758-98-7	7758987	6253	Pest_312	6017	160	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				100%	-7.2	-7.2	-8.9
Prometryn		7287-19-6	7287196	87	Pest_228	6018	241	132.0	2.5E-03	2.4E+01	5.4E+03	0	9.9	2.2E-09	3.5E-08	1.1E-07				100%	-7.3	-7.2	-9.0
Propachlor		1918-16-7	1918167	520	Pest_107	6019	212	85.6	2.5E-02	7.5E+02	2.6E+02	0	15	7.1E-08	1.1E-07	3.5E-07				100%	-7.3	-7.2	-9.0
Imidacloprid		138261-41-3	138261413	443	Pest_68	6020	256	156.0	2.2E-04	2.1E+03	3.6E+00	11.1	13	6.3E-08	3.5E-08	1.1E-07				100%	-6.9	-7.2	-8.8
Maneb		12427-38-2	12427382	6283	Pest_368	6021	265	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				100%	-7.3	-7.2	-9.0
Zineb		12122-67-7	12122677	6453	Pest_435	6022														100%	-7.3	-7.2	-9.0
Glufosinate		51276-47-2	51276472	4969	Pest_359	6023	181	272.1	1.5E-08	3.5E+03	3.2E-05	1.86	4.25	1.1E-06	1.1E-07	3.5E-07				100%	-6.8	-7.3	-9.8
Captan		133-06-2	133062	425	Pest_58	6024	301	183.5	3.4E-06	1.2E+02	5.5E+02	0	16	8.7E-08	3.5E-08	3.5E-08				100%	-6.8	-7.3	-8.8
Azoxystrobin		131860-33-8	131860338	423	Pest_56	6025	403	228.1	6.6E-08	2.3E+00	3.8E+01	0	13	1.0E-07	3.5E-08	1.1E-07				100%	-6.9	-7.4	-9.0
Alachlor		15972-60-8	15972608	497	Pest_86	6026	270	128.5	2.7E-03	1.7E+02	2.3E+03	0	0	7.1E-08	3.5E-08	1.1E-07				100%	-7.4	-7.4	-8.7
Fosetyl		15845-66-6	15845666	4965	Pest_358	6027	110	-11.0	7.4E+00	5.7E+05	2.0E-01	2.4	0	3.5E-06	3.5E-07	1.1E-06				100%	-7.4	-7.4	-10.1
Pyrazophos		13457-18-6	13457186	432	Pest_62	6028	373	87.7	3.0E-05	2.4E+01	6.3E+03	0	13	7.9E-08	1.1E-07	3.5E-07				100%	-7.5	-7.4	-9.2
Iprodione		36734-19-7	36734197	616	Pest_163	6029	330	233.6	2.0E-08	9.9E+01	7.1E+02	13	0	9.5E-08	3.5E-08	1.1E-07				100%	-7.5	-7.5	-9.2
Dimethenamid-P		163515-14-8	163515148	502	Pest_88	6030	276	138.6	4.0E-03	7.1E+03	3.7E+02	0	0	1.2E-07	1.1E-07	3.5E-07				100%	-7.5	-7.5	-9.2
Dimethoate		60-51-5	60515	753	Pest_204	6031	229	86.0	5.5E-03	3.0E+03	5.2E+00	15.1	14	6.9E-08	1.1E-07	1.1E-06				100%	-7.5	-7.5	-9.2
Copper oxide		1317-38-0	1317380	6421	Pest_309	6032														100%	-7.5	-7.5	-9.2
Copper hydroxide		20427-59-2	20427592	6420	Pest_308	6033														100%	-7.5	-7.5	-9.2
Oxine-copper		10380-28-6	10380286	6302	Pest_389	6034	352	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				100%	-7.5	-7.5	-9.2
Copper carbonate		1184-64-1	1184641	6251	Pest_306	6035	124	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				100%	-7.5	-7.5	-9.2

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Cyanazine		21725-46-2	21725462	535	Pest_116	6036	241	151.6	2.0E-04	6.8E+00	3.2E+02	0	13	2.2E-09	1.1E-07	1.1E-07				100%	-7.6	-7.5	-9.3
Epoxyconazole		133855-98-8	133855988	4924	Pest_338	6037	330	172.6	3.7E-05	2.5E+01	3.0E+03	0	12.8	1.1E-08	3.5E-09	1.1E-08				100%	-7.3	-7.6	-8.7
Dodine		2439-10-3	2439103	6262	Pest_336	6038	287	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				100%	-7.6	-7.6	-9.3
Triflumizole		68694-11-1	68694111	802	Pest_219	6039	346	150.9	2.3E-04	3.3E+00	3.2E+01	0	11	1.3E-08	3.5E-08	1.1E-07				100%	-7.8	-7.6	-8.7
Methomyl		16752-77-5	16752775	506	Pest_90	6040	162	2.7	3.4E+00	1.1E+04	4.1E+00	13.9	15	1.3E-07	3.5E-08	3.5E-07				100%	-7.8	-7.6	-9.2
Dimethachlor		50563-36-5	50563365	663	Pest_179	6041	256	120.6	5.7E-02	2.3E+03	2.1E+02	0	15	7.8E-08	3.5E-08	1.1E-07				100%	-7.7	-7.6	-9.1
Difenzoquat		49866-87-7	49866877	4903	Pest_326	6042	249	143.8	6.5E-05	1.6E-01	5.1E+00	0	0	1.1E-07	1.1E-08	3.5E-08				100%	-7.9	-7.6	-9.3
Oxamyl		23135-22-0	23135220	549	Pest_124	6043	219	95.0	7.8E-03	1.9E+04	6.3E-02	13.5	16	1.7E-07	3.5E-08	3.5E-07				100%	-7.3	-7.6	-9.5
Metribuzin		21087-64-9	21087649	531	Pest_113	6044	214	150.4	6.9E-04	2.7E+03	3.1E+01	0	6	2.7E-08	1.1E-07	3.5E-07				100%	-7.1	-7.6	-8.8
Paraquat		4685-14-7	4685147	5085	Pest_391	6045	186	84.8	3.3E-02	1.4E+04	2.8E-01	0	0	3.5E-07	3.5E-08	1.1E-07				100%	-7.5	-7.6	-9.8
Thiacloprid		111988-49-9	111988499	6	Pest_20	6046	253	150.4	1.5E-04	4.1E+02	2.1E+02	0	7.02	2.2E-08	3.5E-08	1.1E-07				100%	-7.2	-7.6	-8.8
Carbendazim		10605-21-7	10605217	3	Pest_299	6047	191	149.7	7.3E-07	1.0E+03	3.5E+01	10	9.5	1.2E-08	1.1E-07	3.5E-07				100%	-7.1	-7.7	-8.7
Bentazone		25057-89-0	25057890	39	Pest_290	6048	240	173.0	3.4E-05	2.9E+03	4.7E+01	2.9	0	1.8E-07	1.1E-07	3.5E-07				100%	-7.1	-7.7	-9.4
Trichlorfon		52-68-6	52686	677	Pest_183	6049	257	66.1	9.3E-03	1.7E+05	2.6E+00	7.76	0	3.7E-08	1.1E-08	3.5E-08				100%	-7.3	-7.7	-9.1
Folpet		133-07-3	133073	426	Pest_59	6050	297	188.7	1.9E-06	3.0E+00	6.9E+02	0	16	2.6E-07	3.5E-07	1.1E-06				100%	-7.0	-7.7	-9.1
Dicloran		99-30-9	99309	1085	Pest_276	6051	207	113.8	1.6E-03	3.4E+02	5.8E+02	0	0	2.2E-09	3.5E-08	1.1E-07				100%	-7.5	-7.7	-8.6
Propyzamide		23950-58-5	23950585	556	Pest_128	6052	256	152.9	1.4E-04	1.6E+01	3.7E+03	14.4	16	2.4E-08	1.1E-08	3.5E-08				100%	-7.7	-7.7	-8.9
Chlorothalonil		1897-45-6	1897456	516	Pest_102	6053	266	131.5	6.3E-05	7.4E-01	4.6E+03	0	0	2.2E-09	3.5E-08	1.1E-07				100%	-7.9	-7.7	-8.5
Thiabendazole		148-79-8	148798	476	Pest_77	6054	201	181.1	8.3E-08	2.6E+02	1.0E+02	13.2	9	7.2E-09	3.5E-08	1.1E-07				100%	-7.2	-7.8	-8.8
Diquat		2764-72-9	2764729	4912	Pest_334	6055	184	95.3	2.0E-02	9.2E+03	2.1E-01	0	0	1.1E-06	1.1E-07	3.5E-07				100%	-7.6	-7.8	-10.3
Thiophanate-methyl		23564-05-8	23564058	552	Pest_126	6056	342	185.3	1.3E-06	1.0E+02	1.3E+01	7.29	13	1.4E-08	1.1E-07	3.5E-07				100%	-7.3	-7.8	-8.9
Ethofumesate		26225-79-6	26225796	573	Pest_136	6057	286	141.8	1.2E-03	1.2E+02	7.8E+02	0	0	1.1E-07	1.1E-07	3.5E-07				100%	-7.7	-7.9	-9.2
Flutriafol		76674-21-0	76674210	875	Pest_236	6058	301	164.5	2.7E-06	2.7E+02	3.3E+02	13.4	13	2.2E-09	3.5E-08	1.1E-07				100%	-7.3	-7.9	-8.8
Aclonifen		74070-46-5	74070465	835	Pest_233	6059	265	160.0	3.3E-04	2.4E+01	7.6E+03	0	0	4.2E-09	3.5E-08	1.1E-07				100%	-7.7	-7.9	-8.6
Oryzalin		19044-88-3	19044883	517	Pest_103	6060	346	208.7	4.0E-07	5.8E+00	5.4E+02	9.38	0	1.8E-08	3.5E-08	1.1E-07				100%	-7.3	-7.9	-9.0
Mecoprop-P		16484-77-8	16484778	503	Reach_2421	6061	215	102.3	6.1E-02	4.9E+02	8.7E+02	3.05	0	3.7E-09	1.1E-07	1.1E-06				100%	-8.0	-7.9	-8.5
S-Metolachlor		87392-12-9	87392129	1115	Pest_411	6062	284	136.1	6.7E-01	2.2E+02	1.7E+03	0	15	6.8E-08	3.5E-08	1.1E-07				100%	-8.0	-7.9	-8.7
Vamidothion		2275-23-2	2275232	543	Pest_119	6063	287	85.0	1.8E-04	1.5E+03	1.1E+00	13.7	15	3.4E-08	3.5E-08	3.5E-07				100%	-7.5	-7.9	-9.2
Chlorthal		2136-79-0	2136790	4873	Pest_303	6064	304	178.1	6.5E-06	6.8E+00	1.3E+02	1.65	0	1.1E-07	3.5E-08	1.1E-07				100%	-7.5	-7.9	-9.5
Flumetsulam		98967-40-9	98967409	1081	Reach_4516	6065	325	190.0	2.0E-07	2.9E+02	3.2E+01	5.02	12	3.7E-09	1.1E-07	3.5E-07				100%	-7.3	-7.9	-8.9
Phenmedipham		13684-63-4	13684634	440	Pest_66	6066	300	126.2	8.9E-05	4.1E+00	1.9E+03	12.9	0	3.3E-08	1.1E-07	3.5E-07				100%	-7.9	-7.9	-8.9
Flufenacet		142459-58-3	142459583	461	Pest_73	6067	363	181.4	5.6E-05	2.6E+00	2.5E+02	0	13	2.0E-08	3.5E-08	1.1E-07				100%	-8.1	-7.9	-9.1
Bromofenoxim		13181-17-4	13181174	422	Pest_55	6068	461	221.3	2.3E-09	6.1E-01	3.5E+03	5.06	0	6.5E-08	3.5E-08	1.1E-07				100%	-7.2	-8.0	-9.2
Sulcotrione		99105-77-8	99105778	1083	Pest_274	6069	329	200.2	1.2E-06	2.8E+02	2.0E+02	3.14	0	2.6E-07	1.1E-07	3.5E-07				100%	-7.3	-8.0	-9.7
1,3-Dichloropropene		542-75-6	542756	1107	Pest_277	6070	111	-72.8	3.0E+03	4.9E+03	1.9E+02	0	0	1.2E-07	1.1E-08	3.5E-08				100%	-8.5	-8.0	-10.0
Fluquinconazole		136426-54-5	136426545	438	Pest_64	6071	376	218.1	3.3E-08	7.5E-02	5.4E+03	0	5	2.4E-08	1.1E-08	3.5E-08				100%	-7.5	-8.0	-9.2
Mesotrione		104206-82-8	104206828	167	Pest_13	6072	339	217.5	1.8E-08	8.0E+02	3.1E+01	2.65	0	2.7E-07	3.5E-08	1.1E-07				100%	-7.5	-8.0	-10.0
Dichlobenil		1194-65-6	1194656	352	Reach_1672	6073	172	52.7	7.8E-02	6.3E+01	6.8E+02	0	0	3.2E-09	1.1E-08	3.5E-08				100%	-8.2	-8.0	-8.9
Methamidophos		10265-92-6	10265926	153	Pest_9	6074	141	14.6	9.1E+00	1.3E+05	1.2E-01	0	0	1.0E-08	3.5E-07	1.1E-06				100%	-8.2	-8.0	-9.1
Heptenophos		23560-59-0	23560590	551	Pest_125	6075	251	72.3	1.2E-01	1.7E+03	2.6E+01	0	0	5.9E-08	3.5E-08	1.1E-07				100%	-8.3	-8.0	-9.4
Pendimethalin		40487-42-1	40487421	628	Pest_170	6076	281	148.1	2.7E-02	1.7E+01	6.6E+04	0	0	3.1E-09	3.5E-08	1.1E-07				100%	-8.1	-8.0	-8.6
DNOC		534-52-1	534521	682	Reach_1332	6077	198	121.2	2.3E-04	4.7E+03	1.9E+02	4.2	0	2.2E-09	3.5E-08	1.1E-07				100%	-7.6	-8.0	-9.0
Fluazinam		79622-59-6	79622596	925	Pest_240	6078	465	190.8	7.3E-06	1.4E-01	1.0E+04	6.19	0	1.5E-08	3.5E-08	1.1E-07				100%	-8.1	-8.1	-8.9
Simazine		122-34-9	122349	15	Pest_43	6079	202	112.1	1.2E-03	3.4E+01	2.5E+02	0	12.3	2.7E-09	1.1E-07	3.5E-07				100%	-8.1	-8.1	-8.9
Nuarimol		63284-71-9	63284719	773	Pest_207	6080	315	173.3	8.2E-07	5.7E+01	1.5E+03	13.3	12	2.2E-09	3.5E-09	1.1E-08				100%	-7.6	-8.1	-9.0
Mecoprop		93-65-2	93652	108	Pest_264	6081	215	102.3	6.1E-02	4.9E+02	8.7E+02	3.05	0	3.7E-09	1.1E-07	1.1E-06				100%	-8.2	-8.1	-8.7
Acephate		30560-19-1	30560191	596	Pest_147	6082	183	80.1	7.3E-03	6.4E+04	1.3E-01	12.1	0	8.7E-08	3.5E-07	1.1E-06				100%	-7.7	-8.1	-9.7
Linuron		330-55-2	330552	602	Pest_150	6083	249	137.2	1.6E-03	1.2E+02	8.1E+02	0	0	2.2E-09	3.5E-08	1.1E-07				100%	-8.1	-8.1	-9.0
Omethoate		1113-02-6	1113026	295	Pest_18	6084	213	87.0	8.1E-03	3.5E+04	1.6E-01	14	15	9.5E-08	1.1E-07	1.1E-06				100%	-7.7	-8.1	-9.7
Chlorotoluron		15545-48-9	15545489	32	Pest_82	6085	213	118.6	1.2E-03	2.3E+02	3.8E+02	14	15	8.5E-09	3.5E-08	1.1E-07				100%	-7.9	-8.1	-9.1
Tebuconazole		107534-96-3	107534963	221	Pest_16	6086	308	162.9	6.1E-06	2.9E+01	7.8E+03	13.7	12	3.8E-09	3.5E-08	1.1E-07				100%	-7.3	-8.1	-8.9
Monuron		150-68-5	150685	482	Pest_80	6087	199	107.4	1.3E-03	4.1E+02	1.1E+02	14.1	15	8.9E-09	3.5E-08	1.1E-07				100%	-7.9	-8.1	-9.2
Propanil		709-98-8	709988	816	Pest_224	6088	218	131.0	3.8E-03	3.6E+01	7.6E+02	12.9	15	1.0E-07	3.5E-08	1.1E-07				100%	-8.3	-8.1	-9.6
Famoxadone		131807-57-3	131807573	421	Pest_54	6089	374	254.2	1.3E-09	2.1E+00	7.8E+04	0	0	8.6E-09	1.1E-07	3.5E-07				100%	-8.2	-8.1	-9.9
Benzthiazuron		1929-88-0	1929880	522	Pest_109	6090	207	160.3	8.9E-05	7.4E+02	1.3E+02	14.3	14	5.0E-09	3.5E-08	1.1E-07				100%	-7.7	-8.1	-9.1
Vinclozolin		50471-44-8	50471448	661	Pest_178	6091	286	187.7	1.2E-05	4.2E+03	1.1E+03	0	0	1.2E-08	3.5E-08	1.1E-07				100%	-8.2	-8.1	-9.9
Monocrotophos		6923-22-4	6923224	803	Pest_220	6092	223	87.7	3.7E-03	3.5E+04	4.9E-01	11	0	5.7E-08	1.1E-07	1.1E-06				100%	-7.7	-8.1	-9.6
Bitertanol		55179-31-2	55179312	693	Pest_187	6093	337	196.8	1.9E-08	2.0E+01	1.2E+04	14.9	14	1.7E-08	1.1E-08	3.5E-08				100%	-7.4	-8.1	-9.2
Dimethenamid		87674-68-8	87674688	1109	Pest_329	6094	276	138.6	4.0E-03	7.1E+03	3.7E+02	0	0	1.2E-07	1.1E-07	3.5E-07				100%	-7.6	-8.2	-9.6
Prosulfocarb		52888-80-9	52888809	60	Pest_184	6095	251	117.5	6.4E-03	1.4E+01	1.7E+04	0	14.6	2.1E-07	3.5E-08	3.5E-07				100%	-8.3	-8.2	-9.4
Florasulam		145701-23-1	145701231	473	Pest_75	6096	360	194.4	5.8E-07	9.4E+00	1.3E+02	4.72	13	3.0E-09	1.1E-07	3.5E-07				100%	-7.6	-8.2	-9.0
Monolinuron		1746-81-2	1746812	511	Pest_96	6097	215	118.4	5.9E-03	2.1E+02	1.8E+02	0	0	2.2E-09	3.5E-08	1.1E-07				100%	-8.3	-8.2	-9.1
Tolylfluanid		731-27-1	731271	827	Pest_229	6098	347	150.8	2.6E-04	2.2E+00	1.9E+03	0	0	2.2E-08	1.1E-07	3.5E-07				100%	-8.3	-8.2	-9.1
Metoxuron		19937-59-8	19937598	527	Pest_111	6099	229	129.5	1.1E-03	3.5E+02	1.3E+02	14.2	14	5.7E-08	3.5E-08	1.1E-07				100%	-8.0	-8.2	-9.6
Fenarimol		60168-88-9	60168889	747	Pest_202	6100	331	183.3	2.3E-07	1.8E+01	4.2E+03	13.1	12	2.2E-09	3.5E-09	1.1E-08				100%	-7.6	-8.2	-9.2
Dicamba		1918-00-9	1918009	519	Pest_106	6101	221	112.3	7.1E-03	5.0E+02	1.4E+02	2.39	0	9.5E-08	1.1E-07	3.5E-07				100%	-8.2	-8.2	-9.7
Fentin		668-34-8	668348	790	Pest_214	6102	350	94.0	1.0E-02	0.0E+00	3.8E+06	0	0	2.6E-08	3.5E-09	1.1E-08				100%	-8.3	-8.2	-10.0
Fentin acetate		900-95-8	900958	6427	Pest_345	6103														100%	-8.3	-8.2	-10.0
Barium Polysulfide		50864-67-0	50864670	6239	Pest_288	6104	169	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				100%	-8.3	-8.2	-10.0
Fenuron		101-42-8	101428	147	Pest_6	6105	164	93.6	1.0E-02	2.6E+03	2.4E+01	14.3	14	1.2E-08	1.1E-07	3.5E-07				100%	-8.0	-8.2	-9.3
Trifluralin		1582-09-8	1582098	496	Pest_85	6106	335	140.0	1.8E-03	2.8E-01	2.0E+05	0	0	1.8E-08	3.5E-08	1.1E-07				100%	-8.3	-8.2	-8.8
Fenbutatin-oxide		13356-08-6	13356086	6426	Pest_340	6107														100%	-8.3	-8.2	-10.0
Fluometuron		2164-17-2	2164172	534	Pest_115	6108	232	96.3	3.8E-03	1.2E+02	2.2E+02	13.9	15	8.8E-09	3.5E-08	1.1E-07				100%	-8.4	-8.2	-9.2
Metobromuron		3060-89-7	3060897	598	Pest_148	6109	259	131.2	2.2E-03	3.1E+02	3.2E+02	0	0	2.2E-09	3.5E-08	1.1E-07				100%	-8.2	-8.3	-9.2
Fuberidazole		3878-19-1	3878191	622	Pest_166	6110	184	148.6	6.2E-07	4.5E+02	2.3E+02	13.2	11	3.5E-09	1.1E-07	3.5E-07				100%	-7.6	-8.3	-9.1

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Myclobutanil		88671-89-0	88671890	984	Pest_261	6111	289	166.7	3.1E-04	3.7E+00	3.2E+03	0	13	4.6E-09	3.5E-08	1.1E-07				100%	-8.4	-8.3	-9.1
Aldicarb		116-06-3	116063	342	Pest_29	6112	190	28.8	6.4E-01	1.9E+03	2.3E+01	13.7	15	7.6E-08	3.5E-08	3.5E-07				100%	-8.5	-8.3	-9.7
Quinmerac		90717-03-6	90717036	1003	Pest_262	6113	222	144.4	1.8E-05	1.1E+02	7.4E+02	0.51	10	9.7E-08	1.1E-07	3.5E-07				100%	-7.6	-8.3	-9.6
Benomyl		17804-35-2	17804352	513	Pest_98	6114	290	221.7	8.1E-08	3.8E+02	1.7E+02	9.58	11	7.1E-08	1.1E-07	3.5E-07				100%	-7.6	-8.3	-9.7
Bromuconazole		116255-48-2	116255482	343	Pest_30	6115	377	172.7	1.3E-04	2.8E+00	3.5E+03	0	13	2.2E-09	3.5E-08	1.1E-07				100%	-8.4	-8.3	-9.1
Methiocarb		2032-65-7	2032657	528	Pest_112	6116	225	95.1	8.1E-03	9.5E+01	7.4E+02	12.2	0	8.6E-09	1.1E-07	3.5E-07				100%	-8.4	-8.3	-9.1
Propazine		139-40-2	139402	446	Reach_1144	6117	230	115.7	9.7E-04	6.4E+00	1.7E+03	0	12	2.2E-09	3.5E-08	1.1E-07				100%	-8.5	-8.3	-9.1
Fentin hydroxide		76-87-9	76879	1110	Pest_346	6118	367	131.1	1.5E-06	0.0E+00	3.0E+03	0	0	3.4E-09	3.5E-09	1.1E-08				100%	-7.8	-8.3	-9.3
Diuron		330-54-1	330541	46	Reach_1238	6119	233	126.4	6.2E-04	6.4E+01	4.7E+02	13.8	15.6	9.0E-09	3.5E-08	1.1E-07				100%	-8.3	-8.3	-9.3
Hexaconazole		79983-71-4	79983714	930	Pest_241	6120	314	166.8	3.1E-06	1.6E+01	4.6E+03	14.2	13	5.7E-09	3.5E-08	1.1E-07				100%	-7.6	-8.3	-9.2
Clopyralid		1702-17-6	1702176	509	Pest_94	6121	192	106.6	8.9E-03	3.9E+02	4.3E+01	2.1	0	3.0E-08	1.1E-07	3.5E-07				100%	-8.4	-8.3	-9.6
Pirimicarb		23103-98-2	23103982	547	Pest_123	6122	238	112.4	1.5E-02	7.9E+02	2.5E+01	0	10	2.2E-08	1.1E-07	3.5E-07				100%	-8.5	-8.4	-9.5
Fluroxypyr		69377-81-7	69377817	805	Pest_221	6123	255	154.4	2.6E-05	8.2E+02	1.5E+01	2.9	16	2.2E-09	1.1E-07	3.5E-07				100%	-7.8	-8.4	-9.3
Methabenzthiazuron		18691-97-9	18691979	515	Pest_100	6124	221	165.2	1.4E-04	3.1E+02	4.5E+02	14.3	14	5.7E-08	3.5E-08	1.1E-07				100%	-7.9	-8.4	-9.8
Fenfuram		24691-80-3	24691803	562	Pest_131	6125	201	133.9	8.7E-04	1.1E+02	4.2E+02	14.8	14	2.0E-07	1.1E-07	3.5E-07				100%	-8.4	-8.4	-10.2
Triadimenol		55219-65-3	55219653	694	Pest_188	6126	296	152.5	4.4E-06	9.2E+02	8.9E+02	14.8	14	4.7E-09	1.1E-07	3.5E-07				100%	-7.6	-8.4	-9.2
Napropamide		15299-99-7	15299997	5058	Pest_380	6127	271	140.0	3.9E-04	4.2E+01	2.1E+03	0	15.6	1.1E-06	3.5E-08	1.1E-07				100%	-8.3	-8.4	-10.5
Carbaryl		63-25-2	63252	76	Pest_206	6128	201	91.2	7.1E-03	9.0E+01	2.2E+02	12.2	0	3.8E-08	3.5E-08	1.1E-07				100%	-8.6	-8.4	-9.7
Triadimefon		43121-43-3	43121433	639	Pest_176	6129	294	148.6	1.2E-03	8.9E+01	8.7E+02	0	15	2.2E-09	1.1E-07	3.5E-07				100%	-8.3	-8.4	-9.2
Tebuthiuron		34014-18-1	34014181	607	Pest_156	6130	228	163.2	5.8E-05	1.8E+02	6.0E+01	14.3	13	5.7E-08	1.1E-07	3.5E-07				100%	-7.9	-8.4	-9.8
Dithianon		3347-22-6	3347226	604	Pest_153	6131	296	219.0	1.2E-08	2.1E+02	4.4E+02	0	0	1.1E-08	3.5E-07	1.1E-06				100%	-7.5	-8.4	-9.1
Triforine		26644-46-2	26644462	5180	Pest_433	6132	435	222.9	4.7E-08	6.2E+00	1.0E+02	10.4	11.8	3.5E-08	1.1E-08	3.5E-08				100%	-8.0	-8.4	-9.8
Boscalid		188425-85-6	188425856	36	Pest_101	6133	343	221.7	9.2E-09	5.3E-03	1.0E+04	13.3	14.8	8.3E-08	3.5E-08	3.5E-08				100%	-7.9	-8.4	-9.9
Alloxydim-sodium		55635-13-7	55635137	6234	Pest_286	6134	345	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				100%	-8.5	-8.5	-10.2
Diniconazole		83657-24-3	83657243	955	Pest_252	6135	326	170.0	6.0E-07	7.7E+00	8.3E+03	15.6	13	8.4E-09	3.5E-08	1.1E-07				100%	-7.6	-8.5	-9.3
Lenacil		2164-08-1	2164081	114	Pest_114	6136	234	188.1	4.0E-08	1.6E+02	5.5E+02	10.1	0	1.6E-07	3.5E-08	1.1E-07				100%	-7.8	-8.5	-10.1
Dichlorvos		62-73-7	62737	4897	Pest_324	6137	221	18.1	8.4E+00	4.3E+03	4.0E+00	0	0	3.5E-07	3.5E-08	1.1E-07				100%	-8.7	-8.5	-10.3
Flamprop-M		90134-59-1	90134591	4953	Pest_349	6138	322	190.5	1.0E-06	4.3E-01	1.1E+03	3.61	15.9	3.5E-07	3.5E-08	1.1E-07				100%	-8.1	-8.5	-10.4
Flamprop		58667-63-3	58667633	4952	Pest_348	6139	322	190.5	1.0E-06	4.3E-01	1.1E+03	3.61	15.9	3.5E-07	3.5E-08	1.1E-07				100%	-8.1	-8.5	-10.4
Terbumeton		33693-04-8	33693048	606	Pest_155	6140	225	126.8	6.5E-03	8.3E+01	4.0E+03	0	10	2.2E-09	1.1E-07	1.1E-07				100%	-8.6	-8.5	-9.3
Phosphamidon		13171-21-6	13171216	5093	Pest_394	6141	300	82.6	4.4E-03	1.6E+03	2.4E+01	0	0	3.5E-07	1.1E-07	3.5E-07				100%	-8.3	-8.5	-10.5
Demeton-S-methyl		919-86-8	919868	1010	Pest_263	6142	230	40.1	1.6E-01	9.5E+02	1.0E+01	0	0	9.7E-09	1.1E-07	1.1E-06				100%	-8.7	-8.5	-9.4
Dalapon		75-99-0	75990	4884	Pest_319	6143	143	23.1	8.9E+01	7.5E+04	4.8E+01	1.6	0	3.5E-07	1.1E-07	3.5E-07				100%	-8.6	-8.5	-10.3
Sodium-arsenite		7784-46-5	7784465	6328	Pest_415	6144														100%	-8.6	-8.5	-10.3
TCA		650-51-1	650511	1230	Reach_1486	6145	185	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				100%	-8.6	-8.5	-10.3
Naled		300-76-5	300765	594	Pest_145	6146	381	76.4	5.6E-02	4.1E+01	4.0E+01	0	0	2.6E-08	3.5E-08	1.1E-07				100%	-8.7	-8.5	-9.6
Cyproconazole		94361-06-5	94361065	1022	Pest_266	6147	292	158.4	7.6E-06	1.2E+02	1.8E+03	14.6	13	2.7E-08	3.5E-08	3.5E-07				100%	-7.8	-8.5	-9.5
Triticonazole		131983-72-7	131983727	424	Pest_57	6148	318	175.1	4.5E-07	3.5E+01	1.3E+04	15.2	12	5.0E-09	3.5E-08	1.1E-07				100%	-7.6	-8.5	-9.2
Fomesafen		72178-02-0	72178020	824	Pest_226	6149	439	241.6	7.8E-10	2.0E+00	2.6E+03	2.96	0	4.1E-08	3.5E-08	1.1E-07				100%	-7.8	-8.5	-9.7
Chlorbromuron		13360-45-7	13360457	428	Pest_60	6150	294	141.4	7.8E-04	6.1E+01	1.4E+03	0	0	2.2E-09	3.5E-08	1.1E-07				100%	-8.5	-8.5	-9.4
Imazalil		35554-44-0	35554440	614	Pest_162	6151	297	151.8	1.2E-02	8.9E+00	1.3E+04	0	8	1.7E-08	1.1E-08	3.5E-08				100%	-8.7	-8.5	-9.4
Metolachlor		51218-45-2	51218452	56	Pest_180	6152	284	136.1	6.7E-01	2.2E+02	1.7E+03	0	15.5	6.8E-08	3.5E-08	1.1E-07				100%	-8.7	-8.6	-9.4
Dimefuron		34205-21-5	34205215	4905	Pest_328	6153	339	213.9	5.4E-08	1.1E+01	3.7E+02	14	13.8	3.5E-07	3.5E-08	1.1E-07				100%	-8.0	-8.6	-10.5
Propoxur		114-26-1	114261	337	Pest_26	6154	209	68.7	1.1E-01	7.8E+02	7.9E+01	12.2	0	9.7E-09	1.1E-07	3.5E-07				100%	-8.8	-8.6	-9.5
Bupirimate		41483-43-6	41483436	633	Pest_174	6155	316	179.4	1.3E-04	5.1E+01	4.8E+02	0	14	6.7E-08	3.5E-08	1.1E-07				100%	-8.3	-8.6	-10.0
Metosulam		139528-85-1	139528851	1922	Pest_70	6156	419	232.1	1.9E-09	2.9E-01	2.9E+03	5.02	12.3	3.5E-07	3.5E-08	1.1E-07				100%	-7.9	-8.6	-10.4
Methidathion		950-37-8	950378	1025	Pest_268	6157	302	84.3	2.9E-04	1.6E+01	3.8E+01	0	13	3.3E-08	1.1E-07	1.1E-06				100%	-8.6	-8.6	-9.7
Formothion		2540-82-1	2540821	569	Pest_134	6158	257	84.7	1.9E-03	3.1E+03	1.8E+01	0	14	9.0E-08	1.1E-07	1.1E-06				100%	-8.1	-8.6	-10.1
Hymexazol		10004-44-1	10004441	121	Pest_1	6159	99	66.5	8.9E-01	3.2E+04	5.8E-01	7	0	3.5E-07	3.5E-07	1.1E-06				100%	-8.7	-8.6	-10.6
Carbofuran		1563-66-2	1563662	491	Pest_84	6160	221	92.8	7.4E-03	6.4E+02	2.0E+02	12.2	0	8.7E-09	1.1E-07	3.5E-07				100%	-8.6	-8.6	-9.6
Metconazole		125116-23-6	125116236	405	Pest_48	6161	320	172.8	6.6E-03	2.7E+01	1.5E+04	13.7	12	3.1E-09	3.5E-08	1.1E-07				100%	-8.8	-8.7	-9.4
Azinphos-methyl		86-50-0	86500	972	Pest_258	6162	317	87.8	1.8E-05	1.6E+01	3.4E+02	0	14	1.1E-08	1.1E-07	3.5E-07				100%	-8.1	-8.7	-9.6
Fenbuconazole		114369-43-6	114369436	338	Pest_27	6163	337	197.7	2.3E-06	6.4E-01	1.7E+04	0	13	2.2E-09	1.1E-07	1.1E-07				100%	-8.1	-8.7	-9.4
Dinitramine		29091-05-2	29091052	4910	Pest_331	6164	322	163.7	2.0E-04	3.8E+00	9.1E+03	0	0	3.5E-07	3.5E-08	1.1E-07				100%	-8.8	-8.7	-10.3
Triazoxide		72459-58-6	72459586	5175	Pest_429	6165	248	200.1	4.0E-07	4.9E+01	2.8E+01	0	7.93	3.5E-07	3.5E-08	1.1E-07				100%	-8.2	-8.7	-10.8
Ethiofencarb		29973-13-5	29973135	593	Pest_144	6166	225	92.3	6.0E-02	4.0E+02	1.1E+02	11.9	0	4.5E-08	1.1E-07	3.5E-07				100%	-8.9	-8.7	-9.9
Fenamiphos		22224-92-6	22224926	540	Pest_118	6167	303	84.8	1.2E-03	2.2E+01	1.9E+03	0	0	7.7E-08	3.5E-08	1.1E-07				100%	-8.8	-8.7	-10.0
Diflufenican		83164-33-4	83164334	951	Pest_250	6168	394	202.4	5.3E-07	4.8E-01	3.4E+03	13.6	12	2.2E-09	1.1E-07	3.5E-07				100%	-8.0	-8.7	-9.4
Flupoxam		119126-15-7	119126157	1684	Pest_33	6169	461	235.3	1.3E-08	4.4E-01	2.8E+04	14.7	14.4	1.1E-07	3.5E-08	3.5E-08				100%	-7.9	-8.7	-10.1
Thiofanox		39196-18-4	39196184	623	Pest_167	6170	218	41.5	3.8E-01	4.0E+02	1.4E+02	13.7	15	5.7E-08	3.5E-08	3.5E-07				100%	-8.9	-8.7	-9.8
Butocarboxim		34681-10-2	34681102	610	Pest_160	6171	190	13.8	3.1E+00	2.5E+03	1.6E+01	13.7	15	5.6E-08	3.5E-08	3.5E-07				100%	-8.9	-8.7	-9.9
Terbacil		5902-51-2	5902512	5149	Pest_424	6172	217	164.2	3.7E-05	3.9E+02	5.6E+01	5.03	0	3.5E-07	1.1E-07	3.5E-07				100%	-8.2	-8.7	-10.7
Anilazine		101-05-3	101053	141	Pest_2	6173	276	149.4	3.2E-04	7.7E+00	4.4E+03	0	11	2.2E-09	1.1E-08	3.5E-08				100%	-8.9	-8.7	-9.6
Tebufenozide		112410-23-8	112410238	328	Pest_23	6174	352	225.2	1.4E-08	3.3E-01	4.2E+04	0	0	1.2E-07	3.5E-08	1.1E-07				100%	-8.8	-8.8	-10.5
Dichlorprop-P		15165-67-0	15165670	4896	Pest_323	6175	235	110.4	4.5E-03	6.9E+02	1.1E+03	2.97	0	1.1E-06	1.1E-07	1.1E-06				100%	-8.4	-8.8	-10.4
Mefenacet		73250-68-7	73250687	830	Pest_231	6176	298	191.7	3.8E-06	1.8E+01	6.3E+02	0	12	2.1E-08	3.5E-07	1.1E-06				100%	-8.0	-8.8	-9.6
Naptalam		132-66-1	132661	5059	Pest_381	6177	291	227.5	1.2E-08	1.8E+01	2.6E+03	3.41	14.4	3.5E-07	3.5E-08	1.1E-07				100%	-8.0	-8.8	-10.5
Ofurace		58810-48-3	58810483	5077	Pest_384	6178	282	164.7	7.3E-06	5.1E+01	2.5E+01	0	0	3.5E-07	3.5E-08	1.1E-07				100%	-8.4	-8.8	-10.9
Oxadixyl		77732-09-3	77732093	5080	Pest_388	6179	278	173.0	2.3E-05	1.6E+04	2.5E+01	0	0	3.5E-07	1.1E-07	3.5E-07				100%	-8.2	-8.8	-10.8
Metalaxyl-M		70630-17-0	70630170	1113	Pest_375	6180	279	130.5	3.8E-03	1.0E+04	5.0E+01	0	0	9.8E-08	1.1E-07	3.5E-07				100%	-8.3	-8.8	-10.3
Propiconazole		60207-90-1	60207901	748	Pest_203	6181	342	172.9	4.8E-04	3.7E+00	1.3E+04	0	13	5.6E-09	1.1E-07	3.5E-07				100%	-8.9	-8.8	-9.4
Formetanate		22259-30-9	22259309	4963	Pest_357	6182	221	88.3	1.3E-03	1.0E+03	7.6E+00	12.2	6.4	1.1E-06	1.1E-07	3.5E-07				100%	-8.5	-8.8	-11.2
Desmedipham		13684-56-5	13684565	439	Pest_65	6183	300	119.9	1.6E-04	1.3E+01	1.7E+03	12.9	0	3.3E-08	3.5E-07	1.1E-06				100%	-8.5	-8.8	-9.7
Bendiocarb		22781-23-3	22781233	544	Pest_120	6184	223	98.3	1.0E-02	2.5E+03	3.5E+02	12.1	0	3.9E-08	1.1E-07	3.5E-07				100%	-8.5	-8.8	-10.0
Ethirimol		23947-60-6	23947606	555	Pest_127	6185	209	125.3	4.8E-04	9.7E+01	2.5E+03	11.1	9	7.2E-09	3.5E-08	1.1E-07				100%	-8.5	-8.8	-9.7

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
2,4-DB		94-82-6	94826	4327	Pest_279	6186	249	125.3	8.5E-03	1.3E+02	4.0E+03	4.66	0	1.1E-06	1.1E-07	3.5E-07				100%	-9.0	-8.9	-10.6
Dicofol		115-32-2	115322	340	Pest_28	6187	370	148.3	9.2E-06	9.3E-03	6.5E+05	9.69	0	4.4E-09	3.5E-09	1.1E-08				100%	-9.0	-8.9	-9.6
Pymetrozine		123312-89-0	123312890	387	Pest_46	6188	217	178.7	1.8E-06	8.2E+03	7.8E+00	0	10	2.6E-07	3.5E-08	1.1E-07				100%	-8.9	-8.9	-10.6
Dichlorprop		120-36-5	120365	4895	Pest_322	6189	235	110.4	4.5E-03	6.9E+02	1.1E+03	2.97	0	1.1E-06	1.1E-07	1.1E-06				100%	-8.5	-8.9	-10.5
Phosmet		732-11-6	732116	828	Pest_230	6190	317	90.3	4.2E-06	6.6E+01	3.0E+02	0	14	2.6E-07	1.1E-07	3.5E-07				100%	-8.3	-8.9	-10.6
Quintozene		82-68-8	82688	5115	Pest_407	6191	295	119.0	3.6E-03	4.1E-01	1.1E+05	0	0	3.5E-08	1.1E-08	1.1E-08				100%	-9.0	-8.9	-9.6
Quinalphos		13593-03-8	13593038	437	Pest_63	6192	298	85.9	1.1E-03	1.4E+01	1.1E+03	0	13	1.0E-08	1.1E-07	3.5E-07				100%	-9.0	-8.9	-9.7
Oxydemeton-methyl		301-12-2	301122	595	Pest_146	6193	246	86.4	6.4E-05	4.1E+03	1.9E+01	0	0	1.2E-08	3.5E-07	3.5E-06				100%	-8.2	-8.9	-9.7
Ethephon		16672-87-0	16672870	505	Pest_89	6194	144	34.6	2.1E-03	2.0E+05	5.6E-01	2.07	0	6.4E-09	1.1E-08	3.5E-08				100%	-8.6	-8.9	-10.0
Triclopyr		55335-06-3	55335063	698	Pest_191	6195	256	135.2	7.7E-04	3.3E+03	3.4E+02	2.9	0	2.2E-09	1.1E-07	3.5E-07				100%	-8.3	-8.9	-9.7
Dimoxystrobin		149961-52-4	149961524	481	Pest_78	6196	326	206.0	1.0E-07	3.1E+00	2.3E+05	13.1	0	2.6E-07	3.5E-08	1.1E-07				100%	-8.0	-8.9	-10.1
Butralin		33629-47-9	33629479	605	Pest_154	6197	295	148.3	7.4E-04	2.5E+00	1.4E+05	0	0	2.2E-09	3.5E-08	1.1E-07				100%	-8.9	-8.9	-9.5
Quinclorac		84087-01-4	84087014	958	Pest_253	6198	242	151.4	5.3E-06	5.8E+01	9.3E+02	2.38	14	9.0E-08	1.1E-07	3.5E-07				100%	-8.2	-8.9	-10.2
Trietazine		1912-26-1	1912261	518	Pest_105	6199	230	119.6	1.4E-02	1.2E+01	2.8E+03	0	12	1.4E-08	1.1E-07	3.5E-07				100%	-9.1	-9.0	-9.7
Propamocarb		24579-73-5	24579735	5105	Pest_400	6200	188	37.4	3.6E+00	7.0E+04	1.3E+01	11.6	4.24	3.5E-06	3.5E-07	1.1E-06				100%	-9.1	-9.0	-11.2
MCPB		94-81-5	94815	5015	Pest_370	6201	229	117.5	4.1E-03	1.2E+02	3.2E+03	4.68	0	1.1E-06	1.1E-07	1.1E-06				100%	-9.0	-9.0	-10.6
Bromoxynil		1689-84-5	1689845	34	Pest_92	6202	277	119.5	3.1E-04	1.2E+02	2.5E+03	4.2	0	1.7E-08	1.1E-06	3.5E-06				100%	-8.2	-9.0	-9.6
Picoxystrobine		117428-22-5	117428225	5095	Pest_396	6203	367	150.0	6.0E-05	4.9E+00	4.7E+03	0	15.1	1.1E-06	1.1E-07	3.5E-07				100%	-8.8	-9.0	-10.7
Difenoconazole		119446-68-3	119446683	351	Pest_35	6204	406	207.0	2.4E-06	5.2E-01	1.6E+05	0	13	2.2E-09	3.5E-08	1.1E-07				100%	-8.3	-9.0	-9.5
Metalaxyl		57837-19-1	57837191	726	Pest_199	6205	279	130.5	3.8E-03	1.0E+04	5.0E+01	0	0	9.8E-08	1.1E-07	3.5E-07				100%	-8.5	-9.0	-10.5
Iprovalicarb		140923-17-7	140923177	453	Pest_71	6206	320	176.9	2.8E-06	1.1E+01	2.1E+03	9.12	15	6.9E-08	1.1E-07	3.5E-07				100%	-8.3	-9.0	-10.2
Furalaxyl		57646-30-7	57646307	725	Pest_198	6207	301	150.4	2.9E-04	2.7E+02	5.0E+02	0	16	1.1E-07	3.5E-08	1.1E-07				100%	-8.6	-9.0	-10.6
Triazophos		24017-47-8	24017478	557	Pest_129	6208	313	87.5	6.8E-04	4.3E+00	2.3E+03	0	13	1.6E-08	1.1E-07	3.5E-07				100%	-9.2	-9.0	-9.9
Fenitrothion		122-14-5	122145	378	Pest_42	6209	277	85.8	1.0E-02	3.8E+01	2.0E+03	0	0	1.2E-08	1.1E-07	3.5E-07				100%	-9.2	-9.0	-9.8
Pyraclostrobin		175013-18-0	175013180	512	Pest_97	6210	388	205.4	1.1E-07	1.3E+00	2.8E+05	0	13	2.0E-07	1.1E-07	1.1E-07				100%	-8.0	-9.0	-10.0
Pirimiphos-Methyl		29232-93-7	29232937	586	Pest_141	6211	305	89.5	5.0E-03	1.1E+01	1.0E+04	0	11	2.6E-08	1.1E-07	3.5E-07				100%	-9.2	-9.1	-9.8
prothiocarb		19622-08-3	19622083	5109	Pest_403	6212	190	108.6	4.3E-03	4.0E+03	1.1E+01	11.6	4.24	1.1E-06	3.5E-07	1.1E-06				100%	-8.6	-9.1	-11.2
Cycluron		2163-69-1	2163691	4880	Pest_315	6213	198	99.5	3.4E-03	2.9E+02	6.9E+02	14.3	13.9	3.5E-07	1.1E-07	3.5E-07				100%	-8.9	-9.1	-10.8
Ioxynil		1689-83-4	1689834	507	Pest_91	6214	371	135.0	1.8E-05	1.3E+02	8.7E+03	4.2	0	1.7E-08	1.1E-06	3.5E-06				100%	-7.9	-9.1	-9.6
Tetradifon		116-29-0	116290	344	Pest_31	6215	356	173.7	1.3E-05	2.4E-02	1.5E+05	0	0	2.2E-09	3.5E-09	3.5E-09				100%	-9.3	-9.1	-10.0
Bromopropylate		18181-80-1	18181801	4865	Pest_295	6216	428	170.1	9.0E-07	5.4E-01	7.9E+04	9.9	0	1.1E-06	1.1E-07	3.5E-07				100%	-9.1	-9.1	-10.9
Chlorfenapyr		122453-73-0	122453730	380	Pest_44	6217	408	171.8	6.0E-05	1.4E-02	3.2E+05	0	0	1.8E-08	1.1E-07	3.5E-07				100%	-9.1	-9.1	-10.9
Benzoximate		29104-30-1	29104301	4847	Pest_291	6218	364	163.3	5.4E-05	8.8E-01	1.6E+04	0	0	1.1E-06	1.1E-07	3.5E-07				100%	-9.1	-9.1	-10.9
Fenazaquin		120928-09-8	120928098	366	Pest_39	6219	306	170.5	9.7E-05	3.6E-01	5.8E+05	0	11	3.6E-09	1.1E-08	3.5E-08				100%	-9.1	-9.1	-10.9
Fluoroglycofen		77501-60-1	77501601	4959	Pest_354	6220	420	209.0	6.4E-08	2.6E+00	5.2E+03	2.65	0	3.5E-07	3.5E-08	1.1E-07				100%	-8.3	-9.1	-10.8
Haloxyfop		69806-34-4	69806344	810	Pest_222	6221	362	175.7	5.3E-05	8.8E+00	2.4E+03	3.08	14	2.2E-09	1.1E-07	1.1E-06				100%	-8.7	-9.1	-9.6
Prohexadione-calcium		127277-53-6	127277536	6311	Pest_399	6222	462	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				100%	-9.1	-9.1	-10.9
Sodium paranitrophenolate		824-78-2	824782	6327	Pest_414	6223														100%	-9.2	-9.1	-10.9
Sodium 5-nitroguaiacolate		67233-85-6	67233856	6324	Pest_412	6224	191	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				100%	-9.2	-9.1	-10.9
Sodium orthonitrophenolate		824-39-5	824395	6326	Pest_413	6225	161	0.0	0.0E+00	0.0E+00	0.0E+00	0	0	0.0E+00	0.0E+00	0.0E+00				100%	-9.2	-9.1	-10.9
Pyrimethanil		53112-28-0	53112280	681	Pest_186	6226	199	113.5	1.4E-02	9.0E+02	1.5E+03	0	10	9.4E-09	1.1E-07	3.5E-07				100%	-9.0	-9.1	-9.9
Penconazole		66246-88-6	66246886	787	Pest_213	6227	284	132.5	4.8E-03	2.8E+00	4.7E+04	0	12	1.2E-07	3.5E-08	1.1E-07				100%	-9.2	-9.1	-10.1
Chlorfenvinphos		470-90-6	470906	1098	Pest_301	6228	360	85.9	1.3E-03	1.8E+00	1.4E+04	0	0	1.3E-08	3.5E-08	1.1E-07				100%	-9.3	-9.1	-9.9
Phoxim		14816-18-3	14816183	475	Pest_76	6229	298	25.8	1.2E-03	6.3E+00	2.5E+04	0	0	4.6E-08	3.5E-08	1.1E-07				100%	-9.2	-9.1	-10.1
Benazolin		3813-05-6	3813056	116	Pest_165	6230	244	175.1	6.3E-06	1.1E+03	1.2E+02	2.87	0	1.0E-08	1.1E-07	3.5E-07				100%	-8.5	-9.2	-10.1
Fenoxaprop-P		113158-40-0	113158400	335	Pest_25	6231	334	197.8	1.0E-06	3.5E+01	1.5E+04	3.1	15	1.5E-08	3.5E-08	3.5E-07				100%	-8.2	-9.2	-9.8
Cymoxanil		57966-95-7	57966957	727	Pest_200	6232	198	188.4	2.9E-06	3.6E+04	1.7E+04	9.7	16	4.3E-07	3.5E-08	3.5E-07				100%	-8.2	-9.2	-10.6
Chlorpyrifos		2921-88-2	2921882	585	Pest_140	6233	351	82.9	2.7E-03	2.4E-01	1.3E+05	0	0	1.3E-08	1.1E-07	3.5E-07				100%	-9.3	-9.2	-9.8
Fenpropimorph		67564-91-4	67564914	4949	Pest_344	6234	303	121.3	9.9E-03	6.1E+00	3.2E+05	0	6.67	1.1E-06	1.1E-07	3.5E-07				100%	-9.3	-9.2	-10.6
Parathion		56-38-2	56382	713	Pest_196	6235	291	89.2	4.5E-03	1.5E+01	5.4E+03	0	0	1.1E-08	1.1E-07	3.5E-07				100%	-9.3	-9.2	-9.9
Fluazifop		69335-91-7	69335917	1112	Pest_350	6236	327	162.8	3.7E-05	5.6E+01	3.8E+03	3.09	13	2.2E-09	1.1E-07	1.1E-06				100%	-8.3	-9.2	-9.7
Isoxaben		82558-50-7	82558507	946	Pest_246	6237	332	198.2	5.7E-07	2.6E+00	9.5E+03	14.7	15	2.3E-07	1.1E-07	3.5E-07				100%	-8.3	-9.2	-10.5
Azinphos-ethyl		2642-71-9	2642719	40	Pest_137	6238	345	90.1	7.3E-06	2.5E+00	3.2E+03	0	14.4	1.0E-08	1.1E-07	1.1E-06				100%	-8.6	-9.2	-9.9
Maleic hydrazide		123-33-1	123331	389	Pest_47	6239	112	149.7	4.9E-06	2.0E+05	1.3E-01	5.7	0	2.2E-09	3.5E-07	1.1E-06				100%	-8.7	-9.2	-10.2
Clodinafop		114420-56-3	114420563	4877	Pest_304	6240	312	172.8	1.4E-05	4.9E+01	4.2E+02	3.08	13.7	1.1E-06	1.1E-07	3.5E-07				100%	-8.7	-9.3	-11.3
Ethalfluralin		55283-68-6	55283686	695	Pest_189	6241	333	141.9	2.0E-03	6.4E-01	1.7E+05	0	0	3.0E-08	3.5E-08	1.1E-07				100%	-9.4	-9.3	-9.9
Tolclofos-methyl		57018-04-9	57018049	718	Pest_197	6242	301	32.8	8.5E-03	1.5E+00	5.9E+04	0	0	1.3E-08	1.1E-07	3.5E-07				100%	-9.4	-9.3	-9.9
Isopropalin		33820-53-0	33820530	4982	Pest_365	6243	309	152.0	3.9E-05	6.6E+00	6.3E+05	0	0	3.5E-07	3.5E-08	1.1E-07				100%	-8.7	-9.3	-10.4
Acifluorfen		50594-66-6	50594666	4828	Pest_283	6244	362	185.9	5.3E-06	1.0E+00	1.5E+04	2.2	0	3.5E-07	3.5E-08	1.1E-07				100%	-8.9	-9.3	-10.9
EPTC		759-94-4	759944	869	Reach_1529	6245	189	60.5	5.0E-01	1.6E+02	1.0E+03	0	14	2.6E-07	3.5E-08	3.5E-07				100%	-9.4	-9.3	-10.4
Malathion		121-75-5	121755	374	Pest_41	6246	330	-23.6	1.7E-02	3.2E+02	1.9E+02	0	0	1.4E-07	3.5E-07	3.5E-06				100%	-9.4	-9.3	-10.5
Flusilazole		85509-19-9	85509199	967	Pest_256	6247	315	143.6	2.5E-03	1.7E+00	7.8E+04	0	12	2.2E-09	1.1E-07	3.5E-07				100%	-9.4	-9.3	-9.9
Phosalone		2310-17-0	2310170	546	Pest_122	6248	368	89.0	1.5E-05	3.0E-01	1.9E+04	0	15	9.8E-09	1.1E-07	3.5E-07				100%	-9.2	-9.3	-9.9
Diazinon		333-41-5	333415	47	Pest_152	6249	304	87.6	7.2E-03	3.9E+00	7.2E+03	0	12.4	1.4E-08	1.1E-07	3.5E-07				100%	-9.5	-9.3	-10.0
Zoxamide		156052-68-5	156052685	490	Pest_83	6250	337	191.6	8.7E-07	1.5E+00	2.2E+04	12.8	0	4.5E-08	3.5E-08	3.5E-08				100%	-8.7	-9.3	-10.5
Dichlofluanid		1085-98-9	1085989	241	Pest_17	6251	333	140.6	4.0E-04	6.7E+00	5.2E+02	0	0	2.3E-08	1.1E-07	3.5E-07				100%	-9.5	-9.3	-10.3
Thiobencarb		28249-77-6	28249776	580	Pest_138	6252	258	122.3	8.3E-03	1.6E+01	7.9E+03	0	15	1.6E-07	3.5E-08	3.5E-07				100%	-9.5	-9.4	-10.6
Prochloraz		67747-09-5	67747095	797	Pest_217	6253	377	213.1	2.1E-06	1.2E+00	1.3E+04	0	8	1.8E-07	1.1E-07	3.5E-07				100%	-8.6	-9.4	-10.6
Propaquizafop		111479-05-1	111479051	303	Pest_19	6254	444	228.0	2.2E-07	2.1E-01	3.9E+04	0	14	1.2E-07	3.5E-08	3.5E-07				100%	-8.5	-9.4	-10.4
Parathion-Methyl		298-00-0	298000	5086	Pest_392	6255	263	79.7	1.5E-02	9.4E+01	5.6E+02	0	0	1.1E-06	1.1E-07	3.5E-07				100%	-9.6	-9.4	-11.3
Kresoxim-Methyl		143390-89-0	143390890	470	Pest_74	6256	313	137.4	1.7E-04	4.2E+00	7.6E+05	0	0	7.1E-07	1.1E-07	3.5E-07				100%	-9.1	-9.4	-10.5
Benfuracarb		82560-54-1	82560541	947	Pest_247	6257	411	164.0	9.3E-05	3.0E+00	1.1E+04	0	7	3.1E-08	1.1E-07	3.5E-07				100%	-9.3	-9.4	-10.2
Mevinphos		7786-34-7	7786347	5035	Pest_378	6258	224	28.1	4.7E-01	1.6E+04	5.8E+00	0	0	3.5E-06	3.5E-07	1.1E-06				100%	-9.5	-9.4	-11.8
Bromacil		314-40-9	314409	4864	Pest_294	6259	261	175.8	1.5E-05	6.8E+02	4.8E+01	5.07	0	1.1E-06	3.5E-07	1.1E-06				100%	-8.8	-9.4	-11.4
Cyprodinil		121552-61-2	121552612	371	Pest_40	6260	225	126.5	5.3E-03	3.2E+01	9.8E+03	0	10	6.4E-09	1.1E-07	3.5E-07				100%	-9.5	-9.4	-10.0

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Thiamethoxam		153719-23-4	153719234	487	Pest_81	6261	292	163.7	5.4E-05	6.4E+01	6.3E+00	0	12	9.9E-09	3.5E-08	1.1E-07				100%	-9.1	-9.4	-10.5
Desmetryn		1014-69-3	1014693	149	Pest_8	6262	213	122.6	6.1E-03	1.1E+02	6.6E+02	0	10	2.2E-09	3.5E-08	1.1E-07				100%	-9.6	-9.4	-10.3
Guazatine		13516-27-3	13516273	4970	Pest_360	6263	356	216.1	2.2E-08	1.1E+01	5.1E+02	0	0	1.1E-06	1.1E-07	3.5E-07				100%	-8.7	-9.4	-11.4
Fenoxycarb		72490-01-8	72490018	825	Pest_227	6264	301	143.5	5.9E-04	1.0E+01	1.7E+04	11.1	0	1.2E-08	1.1E-07	3.5E-07				100%	-9.4	-9.4	-10.1
Monalide		7287-36-7	7287367	5040	Pest_379	6265	240	139.3	1.4E-03	6.9E+00	1.2E+04	13.2	14.1	1.1E-06	1.1E-07	3.5E-07				100%	-9.6	-9.5	-11.1
Tebutam		35256-85-0	35256850	5143	Pest_420	6266	233	95.6	6.1E-02	2.2E+01	3.1E+03	0	14.8	3.5E-07	1.1E-07	3.5E-07				100%	-9.6	-9.5	-10.6
Thidiazuron		51707-55-2	51707552	5158	Pest_426	6267	220	175.9	9.0E-06	1.0E+03	1.3E+02	14.3	13.9	1.1E-06	3.5E-07	1.1E-06				100%	-8.7	-9.5	-11.3
Fluorodifen		15457-05-3	15457053	4958	Pest_353	6268	328	150.4	2.7E-04	1.7E+00	6.5E+03	0	0	1.1E-06	3.5E-08	1.1E-07				100%	-9.7	-9.5	-11.4
Tetraconazole		112281-77-3	112281773	323	Pest_22	6269	372	133.9	1.1E-02	5.0E-01	1.8E+04	0	12	2.2E-09	1.1E-08	3.5E-08				100%	-9.6	-9.5	-10.2
Endosulfan		115-29-7	115297	4921	Pest_337	6270	407	166.5	1.7E-04	7.6E-02	3.2E+03	0	0	3.5E-08	1.1E-08	3.5E-08				100%	-9.6	-9.5	-10.5
Neburon		555-37-3	555373	5063	Pest_382	6271	275	142.7	3.7E-04	9.3E+00	1.4E+04	13.8	15.6	3.5E-07	1.1E-07	3.5E-07				100%	-9.5	-9.5	-10.9
Propham		122-42-9	122429	5107	Pest_401	6272	179	36.0	6.3E-01	8.5E+02	4.6E+02	13.2	0	3.5E-07	1.1E-07	3.5E-07				100%	-9.7	-9.5	-11.1
Thiometon		640-15-3	640153	775	Pest_208	6273	246	-12.2	2.0E-01	7.8E+01	1.2E+03	0	0	1.1E-08	1.1E-07	1.1E-06				100%	-9.7	-9.6	-10.2
Quizalofop		76578-12-6	76578126	5116	Pest_408	6274	345	209.7	5.7E-08	1.6E+01	3.7E+03	3.1	14.3	1.1E-06	3.5E-08	3.5E-07				100%	-8.7	-9.6	-11.3
Mepiquat		15302-91-7	15302917	5017	Pest_372	6275	114	123.3	1.7E-03	2.8E+05	1.5E-01	0	0	1.1E-06	3.5E-08	1.1E-07				100%	-9.2	-9.6	-12.1
Phosthiazate		98886-44-3	98886443	5094	Pest_395	6276	283	87.2	7.7E-04	9.5E+01	3.0E+02	0	0	1.1E-06	1.1E-07	1.1E-06				100%	-9.3	-9.6	-11.4
Methoprotryne		841-06-5	841065	959	Pest_254	6277	271	155.3	1.8E-04	1.6E+02	1.1E+03	0	10	3.7E-08	1.1E-07	1.1E-07				100%	-9.1	-9.6	-10.8
Benfluralin		1861-40-1	1861401	514	Pest_99	6278	335	140.0	2.4E-03	2.2E-01	2.0E+05	0	0	2.4E-09	3.5E-08	1.1E-07				100%	-9.7	-9.6	-10.1
Bifenox		42576-02-3	42576023	4851	Pest_293	6279	342	176.7	7.2E-05	1.0E+00	1.4E+04	0	0	1.1E-06	3.5E-08	1.1E-07				100%	-9.7	-9.6	-11.4
Fonofos		944-22-9	944229	1023	Pest_267	6280	246	0.7	7.3E-02	1.1E+01	1.0E+04	0	0	1.0E-08	3.5E-08	1.1E-07				100%	-9.7	-9.6	-10.2
Diflubenzuron		35367-38-5	35367385	612	Pest_161	6281	311	212.5	1.8E-08	4.2E-01	3.9E+03	8.65	0	2.9E-08	3.5E-08	1.1E-07				100%	-8.9	-9.6	-10.7
Chlozolinate		84332-86-5	84332865	3860	Pest_255	6282	332	205.8	1.2E-06	4.7E+01	1.7E+02	0	0	1.1E-06	1.1E-07	3.5E-07				100%	-9.0	-9.6	-11.7
Trifloxystrobine		141517-21-7	141517217	5178	Pest_431	6283	408	158.5	7.5E-06	1.4E-01	4.2E+06	0	0	1.1E-06	1.1E-07	3.5E-07				100%	-9.3	-9.6	-10.7
Difenoxuron		14214-32-5	14214325	4902	Pest_325	6284	286	176.2	3.9E-06	3.3E+01	3.3E+03	14.3	13.9	1.1E-06	1.1E-07	3.5E-07				100%	-8.8	-9.6	-11.4
Nitrothal-isopropyl		10552-74-6	10552746	176	Pest_14	6285	295	94.3	5.2E-03	1.4E+01	2.0E+03	0	0	2.3E-07	1.1E-07	3.5E-07				100%	-9.8	-9.6	-11.0
Clomazone		81777-89-1	81777891	941	Pest_244	6286	240	132.4	9.3E-01	3.3E+02	7.2E+02	0	0	1.0E-08	3.5E-08	1.1E-07				100%	-9.7	-9.6	-10.4
Foramsulfuron		173159-57-4	173159574	510	Pest_95	6287	452	314.6	4.0E-15	9.8E+02	1.5E-01	3.31	14	5.6E-08	3.5E-08	1.1E-07				100%	-9.2	-9.6	-11.1
Isofenphos		25311-71-1	25311711	567	Pest_133	6288	345	59.3	1.4E-03	1.3E+00	2.5E+04	0	0	2.3E-07	1.1E-07	3.5E-07				100%	-9.8	-9.6	-10.8
Pyridate		55512-33-9	55512339	701	Pest_193	6289	379	220.3	1.3E-06	8.7E-03	5.4E+05	0	11	6.7E-08	1.1E-07	3.5E-07				100%	-9.3	-9.6	-10.3
Cyclanilide		113136-77-9	113136779	334	Pest_24	6290	274	186.8	1.8E-06	4.8E+01	6.9E+01	3.38	0	2.2E-09	1.1E-07	3.5E-07				100%	-9.1	-9.6	-10.5
Molinate		2212-67-1	2212671	537	Pest_117	6291	187	69.6	2.8E-01	3.3E+01	8.1E+02	0	14	1.7E-08	3.5E-07	1.1E-06				100%	-9.8	-9.6	-10.2
Trinexapac-Ethyl		95266-40-3	95266403	1026	Pest_269	6292	252	147.1	1.7E-05	4.8E+02	4.3E+00	4.83	0	8.6E-08	3.5E-07	1.1E-06				100%	-9.1	-9.6	-11.2
Cypromazine		66215-27-8	66215278	4881	Pest_318	6293	166	140.9	1.5E-04	7.9E+04	9.1E+00	0	8.7	1.1E-07	1.1E-07	3.5E-07				100%	-9.2	-9.7	-11.3
Amitraz		33089-61-1	33089611	603	Pest_151	6294	293	132.3	3.5E-04	6.5E-01	3.5E+05	0	10	3.3E-08	3.5E-08	1.1E-07				100%	-9.6	-9.7	-10.4
Fenthion		55-38-9	55389	699	Pest_192	6295	278	11.3	1.8E-02	1.0E+01	1.2E+04	0	0	1.3E-08	3.5E-07	1.1E-06				100%	-9.8	-9.7	-10.3
Ametryn		834-12-8	834128	953	Reach_1562	6296	227	130.6	5.7E-03	1.8E+02	2.1E+03	0	10	2.2E-09	1.1E-07	1.1E-07				100%	-9.7	-9.7	-10.5
Fenothiocarb		62850-32-2	62850322	4946	Pest_341	6297	253	121.3	4.5E-03	7.1E+01	1.9E+03	0	14.4	1.1E-06	1.1E-07	3.5E-07				100%	-9.8	-9.7	-11.5
Fenamidone		161326-34-7	161326347	499	Pest_87	6298	311	199.9	2.5E-07	7.7E-01	2.8E+03	0	6	2.5E-09	3.5E-07	1.1E-06				100%	-8.8	-9.7	-10.2
Amidosulfuron		120923-37-7	120923377	365	Pest_38	6299	369	236.6	7.1E-09	8.3E+02	5.1E-02	3.9	12	4.5E-08	1.1E-07	3.5E-07				100%	-9.2	-9.7	-11.1
Nicosulfuron		111991-09-4	111991094	319	Pest_21	6300	410	266.2	2.6E-10	1.8E+03	7.1E-02	1.71	9	1.3E-07	3.5E-08	1.1E-07				100%	-9.2	-9.7	-11.5
Chlorpyrifos-Methyl		5598-13-0	5598130	709	Pest_194	6301	323	84.1	9.6E-03	1.5E+00	1.3E+04	0	0	1.5E-08	3.5E-08	3.5E-07				100%	-9.9	-9.7	-10.3
Etridiazole		2593-15-9	2593159	571	Pest_135	6302	248	101.9	8.7E+01	7.6E+01	4.0E+03	0	11	5.7E-09	1.1E-08	3.5E-08				100%	-10.1	-9.7	-11.8
Fenoxaprop		95617-09-7	95617097	4947	Pest_342	6303	334	197.8	1.0E-06	3.5E+01	1.5E+04	3.1	14.9	1.1E-06	3.5E-08	3.5E-07				100%	-8.8	-9.7	-11.3
Terbutryn		886-50-0	886500	104	Pest_260	6304	241	139.6	3.1E-03	1.6E+01	5.9E+03	0	9.9	2.2E-09	3.5E-08	1.1E-07				100%	-9.9	-9.7	-10.5
Sulfosulfuron		141776-32-1	141776321	457	Pest_72	6305	470	317.7	6.5E-14	7.3E-01	9.8E+00	3.81	15	1.3E-08	3.5E-08	1.1E-07				100%	-9.2	-9.7	-10.9
Sulfotep		3689-24-5	3689245	5137	Pest_417	6306	322	-32.3	1.9E-02	6.1E+00	9.5E+03	0	0	3.5E-07	1.1E-07	3.5E-07				100%	-9.9	-9.7	-10.9
Prosulfuron		94125-34-5	94125345	1021	Pest_265	6307	419	230.8	1.8E-08	5.1E-01	3.6E+03	3.9	0	2.1E-08	1.1E-07	3.5E-07				100%	-9.8	-9.8	-11.5
Carboxin		5234-68-4	5234684	673	Pest_181	6308	235	165.9	1.7E-04	4.9E+02	3.1E+01	15.1	14	2.1E-07	1.1E-07	1.1E-06				100%	-9.2	-9.8	-11.4
Quizalofop-P-ethyl		100646-51-3	100646513	5117	Pest_409	6309	373	199.7	5.9E-06	5.2E-01	2.2E+04	0	14.3	1.1E-06	3.5E-08	3.5E-07				100%	-9.5	-9.8	-11.4
Vernolate		1929-77-7	1929777	521	Pest_108	6310	203	70.5	2.3E-01	8.1E+01	3.2E+03	0	14	2.5E-07	3.5E-07	1.1E-06				100%	-9.9	-9.8	-10.8
Flazasulfuron		104040-78-0	104040780	166	Pest_12	6311	407	225.6	1.8E-08	7.4E+00	1.2E+01	1.69	9	1.4E-08	3.5E-08	1.1E-07				100%	-9.3	-9.8	-10.9
Benalaxyl		71626-11-4	71626114	823	Pest_225	6312	325	166.2	3.9E-05	1.9E+00	4.9E+03	0	15	1.1E-07	1.1E-07	3.5E-07				100%	-9.7	-9.8	-11.0
Profenofos		41198-08-7	41198087	631	Reach_2738	6313	374	86.5	1.0E-03	4.1E-01	6.6E+04	0	0	3.9E-09	1.1E-07	3.5E-07				100%	-9.9	-9.8	-10.4
Rimsulfuron		122931-48-0	122931480	383	Pest_45	6314	431	273.2	4.3E-11	2.4E+00	1.1E+00	3.98	13	1.4E-08	1.1E-07	3.5E-07				100%	-9.2	-9.8	-10.9
Dialifos		10311-84-9	10311849	4894	Pest_321	6315	394	90.3	4.6E-06	1.8E+00	1.4E+04	0	15	1.1E-06	1.1E-07	3.5E-07				100%	-9.2	-9.8	-11.4
Cycloxydim		101205-02-1	101205021	144	Pest_4	6316	325	172.3	5.1E-07	1.4E+01	7.6E+03	4.35	0	6.6E-08	3.5E-07	1.1E-06				100%	-8.7	-9.8	-10.6
Chlormephos		24934-91-6	24934916	564	Pest_132	6317	235	-25.2	5.1E-01	8.3E+01	1.1E+03	0	0	1.7E-08	1.1E-07	1.1E-06				100%	-10.0	-9.8	-10.3
Cyanamide		420-04-2	420042	636	Reach_1268	6318	42	-36.1	1.9E+03	2.5E+05	1.5E-01	0	13	7.5E-09	1.1E-07	3.5E-07				100%	-10.0	-9.8	-10.8
Disulfoton		298-04-4	298044	590	Pest_143	6319	274	6.9	4.7E-02	1.3E+01	1.2E+04	0	0	9.9E-09	1.1E-07	1.1E-06				100%	-10.0	-9.8	-10.4
Fenhexamid		126833-17-8	126833178	409	Pest_50	6320	302	187.8	2.6E-07	1.3E+00	5.2E+03	7.7	0	9.8E-09	1.1E-07	3.5E-07				100%	-8.9	-9.8	-10.5
Cycloate		1134-23-2	1134232	4878	Pest_314	6321	215	85.7	7.8E-02	4.3E+01	6.5E+03	0	14.4	1.1E-06	1.1E-07	3.5E-07				100%	-10.0	-9.8	-11.3
Mepronil		55814-41-0	55814410	5018	Pest_373	6322	269	171.3	4.6E-05	3.0E+00	1.7E+04	14.7	13.1	3.5E-07	3.5E-08	1.1E-07				100%	-9.7	-9.8	-11.4
Ethoprophos		13194-48-4	13194484	4930	Pest_339	6323	242	42.2	7.8E-02	5.0E+01	1.4E+03	0	0	1.1E-06	1.1E-07	1.1E-06				100%	-10.0	-9.9	-11.4
Ethion		563-12-2	563122	711	Pest_195	6324	384	15.9	4.7E-04	2.1E-01	1.0E+05	0	0	1.7E-08	1.1E-07	1.1E-06				100%	-9.9	-9.9	-10.5
Phorate		298-02-2	298022	589	Pest_142	6325	260	-2.5	9.4E-02	1.6E+01	4.2E+03	0	0	1.1E-08	1.1E-07	1.1E-06				100%	-10.0	-9.9	-10.4
Chlorpropham		101-21-3	101213	145	Pest_5	6326	214	64.9	4.5E-01	1.5E+02	2.0E+03	13.2	0	1.2E-08	1.1E-07	3.5E-07				100%	-10.0	-9.9	-10.5
Chlorfenson		80-33-1	80331	935	Pest_243	6327	303	149.4	2.5E-04	5.0E+00	1.6E+04	0	0	2.2E-09	1.1E-08	3.5E-08				100%	-10.0	-9.9	-10.7
Oxyfluorfen		42874-03-3	42874033	638	Pest_175	6328	362	156.1	3.1E-03	2.8E-01	1.6E+05	0	0	3.5E-08	1.1E-08	3.5E-08				100%	-10.0	-9.9	-10.5
Carbosulfan		55285-14-8	55285148	696	Pest_190	6329	381	176.0	1.1E-04	4.5E+00	3.7E+05	0	6	5.8E-09	1.1E-07	3.5E-07				100%	-9.4	-9.9	-10.3
Tralkoxydim		87820-88-0	87820880	981	Pest_259	6330	329	180.6	4.9E-08	1.3E+00	7.4E+04	4.7	0	6.0E-08	3.5E-08	1.1E-07				100%	-8.9	-9.9	-10.8
Oxadiargyl		39807-15-3	39807153	626	Pest_169	6331	341	185.7	8.8E-06	8.5E-01	1.3E+04	0	14	7.8E-09	1.1E-07	3.5E-07				100%	-9.6	-9.9	-10.6
Quinoclamine		2797-51-5	2797515	5113	Pest_405	6332	208	126.2	2.3E-04	4.2E+01	3.2E+01	0	11	1.1E-06	3.5E-07	1.1E-06				100%	-9.7	-9.9	-12.0
Lindane		58-89-9	58899	68	Pest_367	6333	291	57.0	6.7E-02	6.3E+00	1.8E+04	0	0	9.5E-09	3.5E-09	1.1E-08				100%	-10.1	-9.9	-10.8
Quinomethionate		2439-01-2	2439012	5114	Pest_406	6334	234	162.9	5.1E-05	3.3E+00	2.3E+03	0	14.5	1.1E-06	1.1E-07	3.5E-07				100%	-9.8	-10.0	-11.8
Acidenzolar		126448-41-7	126448417	4827	Pest_282	6335	196	139.5	3.1E-04	3.7E+02	2.0E+01	3.4	0	3.5E-06	3.5E-07	1.1E-06				100%	-9.5	-10.0	-12.2

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Furathiocarb		65907-30-4	65907304	3457	Pest_211	6336	382	155.2	2.3E-04	3.8E+01	2.7E+04	0	0	1.1E-06	1.1E-07	3.5E-07				100%	-9.6	-10.0	-11.6
Flurochloridone		61213-25-0	61213250	4960	Pest_355	6337	312	134.6	2.2E-03	2.8E+01	2.8E+03	0	0	3.5E-07	1.1E-07	3.5E-07				100%	-10.1	-10.0	-11.5
Tri-allate		2303-17-5	2303175	545	Pest_121	6338	305	95.6	2.4E-02	4.5E+00	3.7E+04	0	15	3.0E-07	1.1E-07	3.5E-07				100%	-10.1	-10.0	-10.9
carbophenothion		786-19-6	786196	898	Pest_237	6339	343	50.3	6.3E-04	1.8E-01	2.8E+05	0	0	9.8E-09	1.1E-07	1.1E-06				100%	-10.0	-10.0	-10.6
Cadusafos		95465-99-9	95465999	1027	Pest_270	6340	270	33.4	4.5E-02	5.5E+00	9.5E+03	0	0	5.7E-09	3.5E-07	1.1E-06				100%	-10.2	-10.0	-10.6
Aldimorph		91315-15-0	91315150	4833	Pest_285	6341	284	103.4	4.9E-03	2.7E-03	7.8E+05	0	6.2	3.5E-07	3.5E-08	1.1E-07				100%	-10.2	-10.0	-11.6
Dinoterb		1420-07-1	1420071	4911	Pest_333	6342	240	139.4	1.6E-04	2.1E+02	4.4E+03	4.2	0	1.1E-06	3.5E-08	1.1E-07				100%	-9.5	-10.0	-12.0
Fluazifop-P-butyl		79241-46-6	79241466	4954	Pest_351	6343	383	149.0	8.9E-04	6.0E-01	2.2E+05	0	12.8	1.1E-06	1.1E-07	3.5E-07				100%	-10.1	-10.0	-11.4
Sethoxydim		74051-80-2	74051802	834	Pest_232	6344	327	161.1	1.5E-06	4.8E+00	9.8E+03	4.35	0	6.4E-08	3.5E-07	1.1E-06				100%	-9.0	-10.1	-10.9
Clethodim		99129-21-2	99129212	1084	Pest_275	6345	360	177.5	3.5E-07	2.1E+00	1.6E+04	4.32	0	2.6E-08	3.5E-07	1.1E-06				100%	-8.9	-10.1	-10.7
Flurtamone		96525-23-4	96525234	4150	Pest_272	6346	333	152.8	4.2E-05	8.0E+01	7.4E+02	0	5.04	1.1E-06	1.1E-07	3.5E-07				100%	-9.5	-10.1	-12.0
Tridemorph		24602-86-6	24602866	2398	Pest_130	6347	298	105.8	1.5E-02	1.3E-03	2.4E+06	0	6.2	1.1E-06	1.1E-07	3.5E-07				100%	-10.3	-10.1	-12.5
Azocyclotin		41083-11-8	41083118	630	Pest_171	6348	436	154.3	5.2E-06	0.0E+00	2.5E+05	0	12	4.8E-09	1.1E-07	3.5E-07				100%	-9.3	-10.1	-10.5
Triflumuron		64628-44-0	64628440	3441	Pest_209	6349	359	222.2	1.8E-08	3.8E-02	1.7E+04	8.51	0	3.5E-07	3.5E-08	1.1E-07				100%	-9.3	-10.1	-11.7
Fenpiclonil		74738-17-3	74738173	4948	Pest_343	6350	237	139.1	1.9E-04	1.2E+01	3.0E+03	14.7	0	1.1E-07	1.1E-08	3.5E-08				100%	-10.2	-10.1	-11.7
Temephos		3383-96-8	3383968	5146	Pest_422	6351	466	86.0	1.1E-05	1.6E-02	1.5E+06	0	0	3.5E-07	1.1E-07	3.5E-07				100%	-9.9	-10.1	-11.1
Oxadiazon		19666-30-9	19666309	526	Pest_110	6352	345	178.7	4.5E-05	1.2E+00	6.5E+04	0	14	5.2E-09	1.1E-07	3.5E-07				100%	-9.9	-10.2	-10.7
Methoxyfenozide		161050-58-4	161050584	5021	Pest_376	6353	368	230.9	4.7E-09	6.7E-01	3.0E+03	0	0	1.1E-06	3.5E-08	1.1E-07				100%	-9.5	-10.2	-12.2
Terbufos		13071-79-9	13071799	416	Pest_51	6354	288	13.8	4.7E-02	2.3E+00	3.1E+04	0	0	1.1E-08	1.1E-07	1.1E-06				100%	-10.4	-10.2	-10.8
Fipronil		120068-37-3	120068373	11	Pest_37	6355	437	208.7	5.1E-10	1.8E-02	1.3E+04	0	0	2.2E-09	3.5E-08	1.1E-07				100%	-9.3	-10.2	-10.9
Spiroxamine		118134-30-8	118134308	347	Pest_32	6356	297	105.8	3.2E-02	5.4E+01	3.2E+05	0	5	3.1E-08	1.1E-07	3.5E-07				100%	-10.1	-10.2	-10.8
Thifensulfuron-methyl		79277-27-3	79277273	918	Pest_238	6357	387	244.1	1.9E-09	2.4E+01	1.9E+01	4.06	0	1.5E-07	1.1E-07	3.5E-07				100%	-9.6	-10.2	-11.9
Teflubenzuron		83121-18-0	83121180	5144	Pest_421	6358	381	218.7	1.3E-08	1.3E-02	4.4E+04	8.65	0	3.5E-07	3.5E-08	1.1E-07				100%	-9.5	-10.3	-11.7
Flutolanil		66332-96-5	66332965	4961	Pest_356	6359	323	168.3	5.4E-05	6.0E-01	4.5E+04	12.6	14.7	1.1E-06	3.5E-08	1.1E-07				100%	-10.4	-10.3	-12.0
Haloxyfop-R		95977-29-0	95977290	4971	Pest_361	6360	362	172.1	1.4E-05	8.8E+00	1.7E+05	3.08	13.7	3.5E-06	1.1E-07	1.1E-06				100%	-9.7	-10.3	-11.8
4-CPA		122-88-3	122883	4795	Pest_280	6361	187	89.0	6.5E-03	2.2E+03	9.3E+01	3.05	0	1.1E-06	1.1E-07	3.5E-07				100%	-10.0	-10.3	-12.5
Bensulfuron-methyl		83055-99-6	83055996	949	Pest_249	6362	410	249.9	6.7E-10	8.4E+00	2.6E+01	5.2	0	2.3E-07	1.1E-07	3.5E-07				100%	-9.7	-10.3	-12.2
Tepraloxydim		149979-41-9	149979419	5148	Pest_423	6363	342	173.0	1.6E-08	3.3E+01	1.8E+03	4.34	0	1.1E-06	3.5E-07	1.1E-06				100%	-9.4	-10.4	-12.0
Chlorbufam		1967-16-4	1967164	4870	Pest_300	6364	224	87.9	1.4E-01	9.5E+00	1.0E+03	13.2	0	1.1E-06	1.1E-07	3.5E-07				100%	-10.5	-10.4	-11.5
Metsulfuron-methyl		74223-64-6	74223646	836	Pest_234	6365	381	241.4	3.8E-09	2.6E+01	1.0E+02	4.06	0	8.8E-08	1.1E-07	3.5E-07				100%	-9.8	-10.4	-11.9
Hexaflumuron		86479-06-3	86479063	971	Pest_257	6366	461	231.1	4.7E-09	4.0E-04	4.4E+05	7.6	0	2.6E-08	3.5E-08	1.1E-07				100%	-9.8	-10.5	-11.1
Chlorsulfuron		64902-72-3	64902723	783	Pest_210	6367	358	227.1	1.6E-08	7.9E+00	1.8E+02	4.06	0	2.8E-08	3.5E-08	3.5E-07				100%	-9.8	-10.5	-11.6
Paclobutrazol		76738-62-0	76738620	5082	Pest_390	6368	294	150.1	2.2E-06	3.9E+01	2.3E+03	13.7	12.5	3.5E-07	3.5E-08	3.5E-07				100%	-9.7	-10.5	-12.1
Flupyrsulfuron		150315-10-9	150315109	2009	Pest_79	6369	451	264.1	1.3E-11	6.7E+00	4.2E+00	1.22	15.3	1.1E-06	1.1E-07	3.5E-07				100%	-10.0	-10.5	-13.0
Cyhexatin		13121-70-5	13121705	419	Pest_52	6370	385	141.3	2.7E-07	0.0E+00	4.3E+06	0	0	5.2E-09	1.1E-07	3.5E-07				100%	-9.6	-10.5	-10.8
Prothiofos		34643-46-4	34643464	2711	Pest_159	6371	345	55.6	1.3E-03	6.8E-02	2.2E+06	0	0	1.1E-06	1.1E-07	1.1E-06				100%	-10.6	-10.6	-11.7
Triasulfuron		82097-50-5	82097505	944	Pest_245	6372	402	249.3	7.4E-10	5.1E+00	2.8E+02	4.59	0	2.6E-08	1.1E-07	3.5E-07				100%	-9.8	-10.6	-11.6
Benfuresate		68505-69-1	68505691	4846	Pest_289	6373	256	133.8	8.7E-03	1.7E+02	6.3E+02	0	0	3.5E-06	3.5E-07	1.1E-06				100%	-10.7	-10.6	-12.4
Mesosulfuron-methyl		208465-21-8	208465218	5020	Pest_374	6374	504	303.9	2.3E-14	1.2E+01	6.3E+00	3.74	0	1.1E-06	1.1E-07	3.5E-07				100%	-10.0	-10.6	-13.0
Fludioxonil		131341-86-1	131341861	420	Pest_53	6375	248	143.4	4.2E-05	1.4E+01	6.8E+03	14.9	0	2.9E-09	1.1E-07	3.5E-07				100%	-9.9	-10.6	-11.2
Azafenidin		68049-83-2	68049832	3505	Pest_218	6376	338	188.0	2.6E-06	5.8E+00	6.5E+04	0	0	1.1E-06	1.1E-07	3.5E-07				100%	-9.7	-10.6	-12.1
Ethoxysulfuron		126801-58-9	126801589	407	Pest_49	6377	398	243.5	4.5E-09	5.3E+00	1.0E+02	8.99	12	2.7E-07	1.1E-07	3.5E-07				100%	-10.0	-10.6	-12.4
Tribenuron-methyl		101200-48-0	101200480	142	Pest_3	6378	395	246.3	3.5E-09	9.0E+00	3.5E+02	4.06	0	7.1E-08	1.1E-07	3.5E-07				100%	-9.9	-10.7	-11.9
Fenpropathrin		39515-41-8	39515418	624	Pest_168	6379	349	64.0	4.2E-04	5.7E-01	4.2E+05	0	0	3.8E-08	1.1E-07	3.5E-07				100%	-10.6	-10.8	-11.4
Flufenoxuron		101463-69-8	101463698	148	Pest_7	6380	489	257.7	3.7E-10	6.5E-05	9.3E+05	7.74	0	1.9E-08	1.1E-07	3.5E-07				100%	-9.8	-10.8	-11.2
Pyridaben		96489-71-3	96489713	1055	Pest_271	6381	365	196.2	3.9E-06	8.5E-02	3.0E+05	0	0	2.2E-08	3.5E-08	1.1E-07				100%	-10.5	-10.8	-11.4
Pyridfenox		88283-41-4	88283414	5110	Pest_404	6382	295	125.9	2.6E+01	6.5E+01	1.6E+04	0	9.36	3.5E-08	1.1E-08	1.1E-08				100%	-11.2	-10.8	-12.8
Beta-Cyfluthrin		68359-37-5	68359375	4849	Pest_292	6383	434	92.7	3.5E-05	3.2E-02	5.5E+05	0	0	1.1E-06	3.5E-08	1.1E-07				100%	-10.9	-10.8	-12.3
Lufenuron		103055-07-8	103055078	158	Pest_11	6384	511	232.2	1.1E-08	3.4E-05	4.1E+06	7.54	0	2.5E-08	3.5E-08	1.1E-07				100%	-10.4	-10.8	-11.4
Norflurazon		27314-13-2	27314132	5073	Pest_383	6385	304	159.3	9.5E-05	2.0E+01	1.5E+02	0	10.8	3.5E-06	1.1E-06	3.5E-06				100%	-10.4	-10.8	-12.6
Cypermethrin		52315-07-8	52315078	1099	Pest_317	6386	416	82.1	1.7E-05	5.9E-02	2.4E+06	0	0	3.9E-08	1.1E-07	3.5E-07				100%	-10.3	-10.8	-11.3
Tridiphane		58138-08-2	58138082	5176	Pest_430	6387	320	106.6	5.2E-02	6.1E-01	1.5E+05	0	0	3.5E-08	3.5E-09	1.1E-08				100%	-11.0	-10.9	-11.9
Tebufenpyrad		119168-77-3	119168773	350	Pest_34	6388	334	200.7	7.3E-06	8.2E-01	5.8E+05	13.4	15	3.0E-08	3.5E-08	1.1E-07				100%	-10.3	-10.9	-11.5
Triapenthenol		76608-88-3	76608883	5174	Pest_428	6389	263	134.2	2.0E-05	1.3E+02	4.8E+03	16	12.2	1.1E-06	1.1E-07	3.5E-07				100%	-10.1	-10.9	-12.7
Deltamethrin		52918-63-5	52918635	679	Pest_185	6390	505	139.5	1.2E-06	9.8E-03	1.5E+06	0	0	3.9E-08	1.1E-07	3.5E-07				100%	-10.4	-10.9	-11.4
Bifenthrin		82657-04-3	82657043	948	Pest_248	6391	423	167.4	5.2E-05	7.1E-03	1.4E+08	0	0	2.0E-07	1.1E-07	3.5E-07				100%	-10.6	-11.0	-11.5
Alpha-cypermethrin		67375-30-8	67375308	1108	Pest_287	6392	416	82.1	1.7E-05	5.9E-02	2.4E+06	0	0	3.9E-08	1.1E-07	3.5E-07				100%	-10.5	-11.0	-11.5
Fenpropidin		67306-00-7	67306007	792	Pest_216	6393	273	103.8	2.9E-02	4.7E+00	2.6E+06	0	4	1.1E-08	3.5E-08	1.1E-07				100%	-11.3	-11.1	-12.4
Permethrin		52645-53-1	52645531	676	Pest_182	6394	391	165.0	1.1E-04	1.0E-01	2.7E+07	0	0	4.4E-08	1.1E-07	3.5E-07				100%	-10.5	-11.2	-11.6
Tralomethrin		66841-25-6	66841256	5167	Pest_427	6395	665	215.5	1.5E-08	7.5E-05	3.6E+07	0	0	1.1E-06	1.1E-07	3.5E-07				100%	-10.6	-11.2	-11.9
Flucythrinate		70124-77-5	70124775	811	Pest_223	6396	451	75.2	1.1E-05	3.3E-03	3.6E+06	0	0	2.6E-08	1.1E-07	3.5E-07				100%	-10.9	-11.2	-11.7
Fenpyroximate		134098-61-6	134098616	429	Pest_61	6397	422	217.7	3.5E-07	3.6E-02	3.7E+05	0	12	3.4E-07	1.1E-07	3.5E-07				100%	-10.6	-11.2	-12.2
Tau-fluvalinate		102851-06-9	102851069	157	Pest_10	6398	503	156.2	2.7E-06	1.1E-03	6.5E+06	0	0	1.7E-08	1.1E-07	3.5E-07				100%	-10.8	-11.2	-11.7
Bioresmethrin		28434-01-7	28434017	581	Pest_139	6399	338	146.3	7.1E-04	2.8E-01	1.3E+07	0	0	5.2E-08	1.1E-07	3.5E-07				100%	-10.7	-11.2	-11.7
Resmethrin		10453-86-8	10453868	1114	Pest_410	6400	338	146.3	7.1E-04	2.8E-01	1.3E+07	0	0	5.2E-08	1.1E-07	3.5E-07				100%	-10.7	-11.2	-11.7
Lambda-Cyhalothrin		91465-08-6	91465086	5001	Pest_366	6401	450	68.7	8.5E-05	1.4E-02	7.1E+06	0	0	1.1E-06	1.1E-07	3.5E-07				100%	-11.2	-11.3	-12.4
Esfenvalerate		66230-04-4	66230044	786	Pest_212	6402	420	83.7	5.5E-06	3.6E-04	5.8E+06	0	0	2.6E-08	1.1E-07	3.5E-07				100%	-11.2	-11.3	-11.9
Fenvalerate		51630-58-1	51630581	1111	Pest_347	6403	420	83.7	5.5E-06	3.6E-04	5.8E+06	0	0	2.6E-08	1.1E-07	3.5E-07				100%	-11.2	-11.3	-11.9
Buprofezin		953030-84-7	953030847	4866	Pest_296	6404	305	151.8	1.1E-04	2.1E-01	2.0E+04	0	12.2	1.1E-06	1.1E-07	3.5E-07				100%	-11.5	-11.3	-12.9
Acrinathrin		101007-06-1	101007061	4829	Pest_284	6405	541	2.9	1.8E-05	1.3E-03	5.4E+06	0	0	3.5E-07	1.1E-07	3.5E-07				100%	-11.3	-11.4	-12.2
Imazaquin		81335-37-7	81335377	4977	Pest_363	6406	311	263.6	4.5E-11	4.4E+00	7.9E+02	1.78	9.99	3.5E-06	3.5E-07	1.1E-06				100%	-10.4	-11.4	-13.1
Iodosulfuron		185119-76-0	185119760	4980	Pest_364	6407	493	279.7	1.1E-12	2.0E+00	2.1E+02	1.82	0	1.1E-06	3.5E-07	1.1E-06				100%	-10.6	-11.5	-13.2
Hexythiazox		78587-05-0	78587050	4974	Pest_362	6408	353	230.6	5.8E-08	2.9E+00	3.7E+05	14	14.2	1.1E-06	1.1E-07	3.5E-07				100%	-10.7	-11.5	-12.8
Primisulfuron		113036-87-6	113036876	5103	Pest_397	6409	454	255.5	4.9E-11	2.6E-01	3.6E+01	2	0	3.5E-06	3.5E-07	1.1E-06				100%	-10.9	-11.6	-13.8
Tefluthrin		79538-32-2	79538322	922	Pest_239	6410	419	105.7	4.0E-02	3.4E-02	1.5E+07	0	0	1.3E-08	1.1E-07	3.5E-07				100%	-11.7	-11.6	-13.1

SUBSTANCE IDENTIFICATION							PHYSICAL AND CHEMICAL SUBSTANCE PROPERTIES										ESTIMATED EMISSIONS						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	MW [g/mol]	Tm [°C]	Pvap25 [Pa]	Sol25 [mg/L]	Kow [-]	pKa1 [-]	pKb1 [-]	kdeg(water) [s^{-1}]	kdeg(sed) [s^{-1}]	kdeg(soil) [s^{-1}]	Tonnage [tpa]	Manuf EU [tpa]	Emission [tpa]	Emission [%]	$logCw_{local}$ [g/L]	$logCw_{fresh}$ [g/L]	$logCw_{coast}$ [g/L]
Flucycloxuron		113036-88-7	113036887	4955	Pest_352	6411	484	291.8	9.1E-12	3.1E-04	3.2E+06	8.58	0	3.5E-07	1.1E-07	1.1E-07				100%	-10.7	-11.6	-12.4
Triflusulphuron		135990-29-3	135990293	5179	Pest_432	6412	478	274.5	5.5E-11	8.1E+00	1.3E+03	2.01	0	3.5E-06	3.5E-07	1.1E-06				100%	-11.0	-12.0	-13.7
Flubenzimine		37893-02-0	37893020	2810	Pest_164	6413	416	155.0	7.7E-05	1.2E-03	4.6E+06	0	9.02	3.5E-06	1.1E-07	3.5E-07				100%	-12.4	-12.3	-13.6
Prohexadione		88805-35-0	88805350	5104	Pest_398	6414	212	142.1	2.3E-04	1.9E+05	1.1E+01	4.19	0	3.5E-06	3.5E-07	1.1E-06				100%	-12.4	-13.0	-15.3
Abamectin		71751-41-2	71751412	1097	Pest_281	6415	873	349.8	1.4E-28	3.3E-04	2.5E+04	12.8	0	1.5E-07	3.5E-07	1.1E-06				100%	-13.0	-13.1	-14.0
Diafenthiuron		80060-09-9	80060099	4893	Pest_320	6416	385	196.4	1.4E-06	4.2E-02	5.6E+07	13	12.6	1.1E-06	3.5E-08	1.1E-07				100%	-12.8	-13.2	-13.9

Table SI-3.

See: Table SI-3.pdf

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]		TP(Cwcoast) [-]
REACH - mono constituent organic substances																			
count							*3667*	*3009*	*3667*	*2101*	*1977*	*123*	*3909*	*3909*	*3909*	*3910*	*3910*	*3.1%*	*3910*
sum or mean																*39%*	*20%*	*96.9%*	*5.2%*
standard deviation							*1.33*	*0.53*		*1.10*	*0.42*		*1.2*	*1.1*	*1.2*				
2.5-p													*-7.7*	*-7.9*	*-9.5*	*6.4E-15*	*1.4E-15*		*8.9E-22*
50-p							*4.38*	*0.62*	*3*	*3.78*	*0.61*	*8*	*-5.6*	*-5.8*	*-7.2*	*8.2E-09*	*3.9E-09*		*2.5E-13*
97.5-p													*-3.4*	*-3.6*	*-4.8*	*3.5E-04*	*1.4E-04*		*8.4E-07*
urea	200-315-5	57-13-6	57136	719	Reach_39	1	6.56	0.97	12	6.20	0.70	20	-1.7	-1.7	-3.4	4.6%	4.1%	4.1%	0.0%
α,α-dimethylbenzyl hydroperoxide	201-254-7	80-15-9	80159	932	Reach_259	2	4.00	0.26	3	3.00	0.26		-2.0	-1.8	-2.7	2.3%	3.7%	7.7%	0.4%
ε-caprolactam	203-313-2	105-60-2	105602	180	Reach_646	3	6.29	0.51	3	5.18	0.42		-2.1	-2.2	-3.6	1.9%	1.4%	8.9%	0.0%
4,4'-isopropylidenediphenol	201-245-8	80-05-7	80057	96	Reach_254	4	3.60	0.84	48	2.23	0.83		-1.9	-2.3	-3.6	2.8%	1.0%	9.8%	0.0%
adipic acid, compound with hexane-1,6-diamine (1:1)	222-037-3	3323-53-3	3323533	5845	Reach_1947	5	5.89	1.03	3	4.91	0.87		-2.1	-2.3	-3.7	1.9%	1.0%	10.7%	0.0%
terephthalic acid	202-830-0	100-21-0	100210	122	Reach_552	6	5.57	0.88	3	4.57	0.88		-1.9	-2.4	-4.0	3.1%	0.8%	11.4%	0.0%
melamine	203-615-4	108-78-1	108781	4	Reach_756	7	5.99	0.77	3	4.99	0.77		-1.6	-2.4	-3.8	5.8%	0.8%	12.2%	0.0%
4,4'-Isopropylidenediphenol, oligomeric reaction products with 1	500-033-5	25068-38-6	25068386	5795	Reach_4051	8	3.66	0.43	3	2.82	0.52		-2.3	-2.6	-3.9	1.0%	0.5%	12.6%	0.0%
2,2',2''-nitrilotriethanol	203-049-8	102-71-6	102716	155	Reach_596	9	6.18	0.62	8	4.55	0.95		-2.1	-2.6	-3.4	1.7%	0.5%	13.0%	0.0%
aniline	200-539-3	62-53-3	62533	765	Reach_64	10	4.82	0.99	55	2.87	1.32	6	-2.6	-2.6	-4.1	0.5%	0.5%	13.4%	0.0%
sodium acrylate	231-209-7	7446-81-3	7446813	6021	Reach_2250	11	3.99	1.56	3	3.04	1.80		-2.4	-2.6	-4.0	0.8%	0.4%	13.8%	0.0%
phenol	203-632-7	108-95-2	108952	252	Reach_765	12	4.75	0.79	210	3.21	0.97	18	-2.9	-2.6	-4.1	0.2%	0.4%	14.1%	0.0%
methanol	200-659-6	67-56-1	67561	793	Reach_84	13	6.29	0.89	23	3.88	1.98	6	-3.0	-2.8	-4.1	0.2%	0.3%	14.3%	0.0%
2-aminoethanol	205-483-3	141-43-5	141435	456	Reach_1162	14	5.35	0.77	15	3.27	0.96	3	-2.8	-2.8	-4.3	0.2%	0.2%	14.5%	0.0%
pentaerythritol	204-104-9	115-77-5	115775	341	Reach_944	15	6.95	0.56	3	5.95	0.56		-2.2	-2.8	-3.9	1.5%	0.2%	14.7%	0.0%
propane-1,2-diol	200-338-0	57-55-6	57556	722	Reach_41	16	6.63	0.76	8	6.41	0.89		-2.4	-2.8	-4.4	0.7%	0.2%	14.9%	0.0%
ethanol	200-578-6	64-17-5	64175	776	Reach_70	17	6.36	0.74	26	4.75	1.52	7	-3.0	-2.9	-4.2	0.1%	0.2%	15.1%	0.0%
but-2-yne-1,4-diol	203-788-6	110-65-6	110656	281	Reach_824	18	5.02	0.50	4	4.13	0.69		-2.4	-2.9	-4.2	0.7%	0.2%	15.3%	0.0%
ethylene	200-815-3	74-85-1	74851	3647	Reach_111	3	4.85	0.24	3	3.85	0.24		-3.2	-2.9	-5.1	0.1%	0.2%	15.4%	0.0%
calcium cyanamide	205-861-8	156-62-7	156627	5721	Reach_1215	4	5.46	1.36	3	3.99	1.63		-2.7	-3.0	-4.3	0.3%	0.2%	15.6%	0.0%
propylidynetrimethanol	201-074-9	77-99-6	77996	890	Reach_192	5	6.97	0.43	5	4.24	0.85		-2.7	-3.0	-4.0	0.4%	0.2%	15.7%	0.0%
benzene	200-753-7	71-43-2	71432	821	Reach_103	6	4.88	0.84	44	4.01	0.91	5	-3.3	-3.0	-5.0	0.1%	0.1%	15.8%	0.0%
[2-(acryloyloxy)ethyl]trimethylammonium chloride	256-176-6	44992-01-0	44992010	5888	Reach_2756	7	4.70	1.05	3	3.70	1.05		-2.7	-3.0	-4.3	0.3%	0.1%	15.9%	0.0%
sodium methanolate	204-699-5	124-41-4	124414	5636	Reach_1078	8	6.82	0.70	3	5.61	0.98		-2.7	-3.0	-4.3	0.3%	0.1%	16.1%	0.0%
acrylamide	201-173-7	79-06-1	79061	911	Reach_226	9	5.12	0.68	28	4.12	0.68		-2.8	-3.0	-4.5	0.3%	0.1%	16.2%	0.0%
etidronic acid	220-552-8	2809-21-4	2809214	578	Reach_1871	10	5.64	0.62	11	3.90	0.72	7	-2.5	-3.0	-3.8	0.7%	0.1%	16.3%	0.0%
cyanuric acid	203-618-0	108-80-5	108805	245	Reach_757	11	5.12	2.00	5	4.60	1.63		-2.5	-3.0	-3.8	0.5%	0.1%	16.4%	0.0%
1,2-dichloroethane	203-458-1	107-06-2	107062	206	Reach_691	12	5.23	0.51	15	4.58	0.96	4	-3.3	-3.0	-4.6	0.1%	0.1%	16.5%	0.0%
adipic acid	204-673-3	124-04-9	124049	400	Reach_1065	13	4.96	0.30	4	4.48	0.77		-2.2	-3.0	-4.6	1.3%	0.1%	16.6%	0.0%
tert-butyl methyl ether	216-653-1	1634-04-4	1634044	33	Reach_1701	14	5.87	0.70	28	4.87	0.70		-3.3	-3.0	-4.5	0.1%	0.1%	16.7%	0.0%
oxydipropanol	246-770-3	25265-71-8	25265718	566	Reach_2562	15	6.70	0.53	5	5.70	0.53		-2.4	-3.0	-4.3	0.8%	0.1%	16.8%	0.0%
trisodium citrate	200-675-3	68-04-2	68042	1232	Reach_89	16	6.16	0.37	3	5.16	0.37		-2.8	-3.1	-4.4	0.2%	0.1%	16.9%	0.0%
propene	204-062-1	115-07-1	115071	1629	Reach_935	17	4.42	0.32	3	3.42	0.32		-3.4	-3.1	-5.4	0.0%	0.1%	17.0%	0.0%
calcium tartrate	221-621-5	3164-34-9	3164349	5841	Reach_1923	18	5.00		1				-2.8	-3.1	-4.4	0.2%	0.1%	17.1%	0.0%
2,2'-iminodi(ethylamine)	203-865-4	111-40-0	111400	299	Reach_854	19	5.46	0.67	7	4.46	0.67		-3.2	-3.1	-3.9	0.1%	0.1%	17.2%	0.0%
2-methylpropan-2-ol	200-889-7	75-65-0	75650	863	Reach_156	20	6.63	0.70	24	5.38	0.70		-3.3	-3.1	-4.1	0.0%	0.1%	17.2%	0.0%
ethane-1,2-diol	203-473-3	107-21-1	107211	216	Reach_700	21	7.18	0.48	11	5.93	1.10	5	-2.7	-3.1	-4.8	0.3%	0.1%	17.3%	0.0%
tetrasodium ethylenediaminetetraacetate	200-573-9	64-02-8	64028	1229	Reach_68	22	5.22	0.72	5	4.51	1.00		-2.9	-3.2	-4.5	0.2%	0.1%	17.4%	0.0%
calcium diformate	208-863-7	544-17-2	544172	5925	Reach_1353	23	6.54	1.38	3	5.07	0.44		-2.9	-3.2	-4.5	0.2%	0.1%	17.4%	0.0%
phthalic anhydride	201-607-5	85-44-9	85449	966	Reach_297	24	5.16	0.94	3	4.74	0.79		-3.2	-3.2	-4.8	0.1%	0.1%	17.5%	0.0%
2,2'-iminodiethanol	203-868-0	111-42-2	111422	300	Reach_856	25	5.21	0.77	18	3.91	0.86	4	-2.6	-3.2	-4.8	0.5%	0.1%	17.5%	0.0%
trimethylammonium chloride	209-810-0	593-81-7	593817	1227	Reach_1396	26	3.37	1.58	5	2.37	1.58		-3.0	-3.2	-4.6	0.1%	0.1%	17.6%	0.0%
citric acid	201-069-1	77-92-9	77929	889	Reach_189	27	5.80	0.44	5	4.80	0.44		-2.2	-3.2	-4.8	1.3%	0.1%	17.6%	0.0%
chloroethylene	200-831-0	75-01-4	75014	845	Reach_123	28	5.45	0.61	6	5.03	1.43		-3.6	-3.2	-5.3	0.0%	0.1%	17.7%	0.0%
1-phenylethanol	202-707-1	98-85-1	98851	4194	Reach_520	29	5.27	0.28	3	4.27	0.28		-3.4	-3.2	-4.8	0.0%	0.1%	17.7%	0.0%
4-methyl-m-phenylene diisocyanate	209-544-5	584-84-9	584849	729	Reach_1384	30	5.26	0.96	4	4.26	0.96		-3.5	-3.3	-4.3	0.0%	0.1%	17.8%	0.0%
diphenyl carbonate	203-005-8	102-09-0	102090	1336	Reach_590	31	3.62	0.46	3	2.80	0.77		-3.5	-3.3	-4.7	0.0%	0.1%	17.8%	0.0%
styrene	202-851-5	100-42-5	100425	125	Reach_557	32	4.25	0.49	11	3.25	0.70	44	-3.5	-3.3	-5.1	0.0%	0.1%	17.9%	0.0%
hexamethylenediamine	204-679-6	124-09-4	124094	1783	Reach_1067	33	4.91	0.50	3	3.91	0.50		-3.2	-3.3	-4.9	0.1%	0.1%	17.9%	0.0%
maleic anhydride	203-571-6	108-31-6	108316	235	Reach_740	34	5.06	0.75	10	4.06	0.75		-3.5	-3.3	-4.8	0.0%	0.0%	18.0%	0.0%
acetic acid	200-580-7	64-19-7	64197	778	Reach_72	35	5.39	0.90	9	4.39	0.75		-2.7	-3.3	-5.0	0.4%	0.0%	18.0%	0.0%
(3-chloro-2-hydroxypropyl)trimethylammonium chloride	222-048-3	3327-22-8	3327228	5846	Reach_1948	36	5.47	0.87	3	5.30	0.82		-3.1	-3.3	-4.7	0.1%	0.0%	18.0%	0.0%
di-''isononyl'' phthalate	249-079-5	28553-12-0	28553120	582	Reach_2621	37	2.74	0.65	11	2.20	1.28	3	-3.2	-3.3	-3.8	0.1%	0.0%	18.1%	0.0%
naphthalene-2-sulphonic acid	204-375-3	120-18-3	120183	12	Reach_990	38	5.28	0.69	6	4.28	0.69		-2.7	-3.3	-4.2	0.4%	0.0%	18.1%	0.0%
2,2'-oxydiethanol	203-872-2	111-46-6	111466	302	Reach_858	39	7.35	0.70	28	6.68	0.48		-2.5	-3.3	-5.1	0.6%	0.0%	18.1%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]		TP(Cwcoast) [-]
potassium formate	209-677-9	590-29-4	590294	1225	Reach_1388	40	5.70	0.77	4	5.16	0.42		-3.1	-3.3	-4.7	0.1%	0.0%	18.2%	0.0%
1,3,5-trioxane	203-812-5	110-88-3	110883	288	Reach_835	41	7.01	0.27	4	6.01	0.27		-3.6	-3.3	-4.3	0.0%	0.0%	18.2%	0.0%
ethylbenzene	202-849-4	100-41-4	100414	124	Reach_556	42	4.24	0.71	15	3.23	0.59	5	-3.6	-3.4	-5.4	0.0%	0.0%	18.2%	0.0%
2,4,6-trichloro-1,3,5-triazine	203-614-9	108-77-0	108770	1489	Reach_755	43	5.69	0.77	3	4.69	0.77		-3.0	-3.4	-4.6	0.1%	0.0%	18.3%	0.0%
chloroacetic acid	201-178-4	79-11-8	79118	915	Reach_231	44	3.90	1.70	6	4.02	1.03		-2.5	-3.4	-5.0	0.6%	0.0%	18.3%	0.0%
4-nitrotoluene	202-808-0	99-99-0	99990	1095	Reach_545	45	4.42	0.70	28	3.33	0.70		-3.6	-3.4	-4.3	0.0%	0.0%	18.3%	0.0%
dimethyl terephthalate	204-411-8	120-61-6	120616	1717	Reach_999	46	4.45	0.34	3	3.43	0.27		-3.2	-3.4	-5.0	0.1%	0.0%	18.4%	0.0%
4-chloroaniline	203-401-0	106-47-8	106478	193	Reach_669	47	3.93	0.78	17	2.04	1.78	8	-3.0	-3.4	-4.2	0.1%	0.0%	18.4%	0.0%
diphenylamine	204-539-4	122-39-4	122394	379	Reach_1028	48	3.08	0.52	11	2.08	0.55	11	-3.3	-3.4	-4.2	0.1%	0.0%	18.4%	0.0%
trisodium nitrilotriacetate	225-768-6	5064-31-3	5064313	1216	Reach_2075	49	6.26	0.66	21	4.50	0.55	3	-3.1	-3.4	-4.7	0.1%	0.0%	18.5%	0.0%
ethylenediamine	203-468-6	107-15-3	107153	211	Reach_696	50	5.17	0.74	12	4.17	0.74	12	-3.6	-3.4	-4.8	0.0%	0.0%	18.5%	0.0%
sodium benzothiazol-2-yl sulphide	219-660-8	2492-26-4	2492264	1207	Reach_1818	51	3.25	0.51	5	2.51	0.66		-3.2	-3.4	-4.8	0.1%	0.0%	18.5%	0.0%
dimethylammonium chloride	208-046-5	506-59-2	506592	5899	Reach_1312	52	4.32		2				-3.2	-3.4	-4.8	0.1%	0.0%	18.5%	0.0%
sodium benzoate	208-534-8	532-32-1	532321	1218	Reach_1329	53	5.13	0.48	11	4.13	0.48	11	-3.2	-3.4	-4.8	0.1%	0.0%	18.6%	0.0%
4-tert-butylphenol	202-679-0	98-54-4	98544	1073	Reach_511	54	3.74	0.84	24	2.74	0.84		-3.6	-3.4	-4.3	0.0%	0.0%	18.6%	0.0%
2-ethoxy-2-methylpropane	211-309-7	637-92-3	637923	77	Reach_1476	55	5.31	0.64	3	4.31	0.64		-3.7	-3.4	-5.2	0.0%	0.0%	18.6%	0.0%
N,N-dimethylformamide	200-679-5	68-12-2	68122	799	Reach_91	56	6.91	0.51	13	5.14	0.90	4	-3.6	-3.5	-4.9	0.0%	0.0%	18.6%	0.0%
butane	203-448-7	106-97-8	106978	1451	Reach_686	57	4.42	0.38	3	3.42	0.38		-3.7	-3.5	-5.8	0.0%	0.0%	18.7%	0.0%
1-methoxypropan-2-ol	203-539-1	107-98-2	107982	226	Reach_724	58	6.70	0.56	4	5.70	0.70		-3.6	-3.5	-4.9	0.0%	0.0%	18.7%	0.0%
propane	200-827-9	74-98-6	74986	3653	Reach_121	59	4.42	0.38	3	3.42	0.38		-3.7	-3.5	-5.8	0.0%	0.0%	18.7%	0.0%
cumene	202-704-5	98-82-8	98828	1076	Reach_518	60	3.92	0.64	9	2.95	0.70		-3.7	-3.5	-5.3	0.0%	0.0%	18.7%	0.0%
cyclohexanone	203-631-1	108-94-1	108941	251	Reach_764	61	5.58	0.70	20	4.71	0.70		-3.7	-3.5	-4.6	0.0%	0.0%	18.7%	0.0%
(Z)-docos-13-enamide	204-009-2	112-84-5	112845	1607	Reach_926	62	2.11		1	1.95			-3.4	-3.5	-4.6	0.0%	0.0%	18.8%	0.0%
bis(2-chloroethoxy)methane	203-920-2	111-91-1	111911	316	Reach_881	63	5.15	0.30	5	4.15	0.30		-3.7	-3.5	-4.4	0.0%	0.0%	18.8%	0.0%
2-nitrotoluene	201-853-3	88-72-2	88722	985	Reach_329	64	4.52	0.70	28	3.60	0.62		-3.7	-3.5	-4.5	0.0%	0.0%	18.8%	0.0%
acrylonitrile	203-466-5	107-13-1	107131	210	Reach_695	65	4.20	0.63	66	2.82	0.41		-3.7	-3.5	-4.6	0.0%	0.0%	18.8%	0.0%
tert-butyl hydroperoxide	200-915-7	75-91-2	75912	867	Reach_166	66	3.92	0.65	3	3.17	1.35		-3.7	-3.5	-4.5	0.0%	0.0%	18.8%	0.0%
acrylic acid	201-177-9	79-10-7	79107	914	Reach_230	67	5.02	1.56	5	3.22	0.68		-3.0	-3.5	-5.1	0.1%	0.0%	18.9%	0.0%
cyclohexanol	203-630-6	108-93-0	108930	250	Reach_763	68	5.68	0.82	6	3.94	0.70		-3.7	-3.5	-4.9	0.0%	0.0%	18.9%	0.0%
methyloxirane	200-879-2	75-56-9	75569	861	Reach_151	69	4.90	0.61	5	3.90	0.61		-3.8	-3.5	-5.2	0.0%	0.0%	18.9%	0.0%
morpholine	203-815-1	110-91-8	110918	290	Reach_837	70	4.99	0.67	11	4.22	0.70	12	-3.7	-3.5	-4.3	0.0%	0.0%	18.9%	0.0%
Propane-1,2-diol, propoxylated	500-039-8	25322-69-4	25322694	568	Reach_4052	71	6.68	0.74	6	6.47	1.27		-2.9	-3.5	-5.0	0.2%	0.0%	18.9%	0.0%
l-(+)-lactic acid	201-196-2	79-33-4	79334	920	Reach_240	72	5.56	0.46	6	4.82	0.52		-2.7	-3.6	-5.1	0.3%	0.0%	18.9%	0.0%
p-phenylenediamine	203-404-7	106-50-3	106503	196	Reach_672	73	3.45	0.90	5	2.45	0.90		-3.1	-3.6	-4.3	0.1%	0.0%	19.0%	0.0%
N,N'-ethylenebis[N-acetylacetamide]	234-123-8	10543-57-4	10543574	175	Reach_2295	74	6.21	0.42	5	5.21	0.42		-2.6	-3.6	-5.1	0.4%	0.0%	19.0%	0.0%
sodium chloroacetate	223-498-3	3926-62-3	3926623	1215	Reach_2003	75	4.20	1.96	6	3.86	1.25		-3.3	-3.6	-4.9	0.0%	0.0%	19.0%	0.0%
p-xylene	203-396-5	106-42-3	106423	189	Reach_665	76	3.96	0.54	16	3.08	0.70	12	-3.8	-3.6	-5.5	0.0%	0.0%	19.0%	0.0%
2-ethylhexanoic acid	205-743-6	149-57-5	149575	479	Reach_1200	77	5.13	0.47	4	4.42	0.29		-3.5	-3.6	-5.2	0.0%	0.0%	19.0%	0.0%
bis(4-chlorophenyl) sulphone	201-247-9	80-07-9	80079	3786	Reach_255	78	3.37	0.22	3	2.37	0.22		-3.7	-3.6	-4.5	0.0%	0.0%	19.0%	0.0%
tetrasodium 4,4'-bis[[4-[bis(2-hydroxyethyl)amino]-6-(4-sulphon	240-521-2	16470-24-9	16470249	5733	Reach_2420	79	5.39	0.64	3	4.39	0.64		-3.3	-3.6	-5.0	0.0%	0.0%	19.0%	0.0%
furfuryl alcohol	202-626-1	98-00-0	98000	1063	Reach_494	80	5.56	0.66	4	4.56	0.66		-3.8	-3.6	-5.0	0.0%	0.0%	19.1%	0.0%
pentasodium (carboxylatomethyl)iminobis(ethylenenitrilo)tetra	205-391-3	140-01-2	140012	1192	Reach_1146	81	5.35	1.00	4	5.19	0.33		-3.4	-3.6	-5.0	0.0%	0.0%	19.1%	0.0%
pentaerythritol tetrakis(3-(3,5-di-tert-butyl-4-hydroxyphenyl)prc	229-722-6	6683-19-8	6683198	6404	Reach_2202	82	5.33	0.29	3	4.33	0.29		-3.4	-3.6	-5.0	0.0%	0.0%	19.1%	0.0%
2-chloroaniline	202-426-4	95-51-2	95512	1031	Reach_431	83	4.04	0.78	9	1.86	1.05		-3.3	-3.6	-4.4	0.1%	0.0%	19.1%	0.0%
butane-1,4-diol	203-786-5	110-63-4	110634	1526	Reach_822	84	6.50	1.28	3	5.50	1.28		-2.9	-3.6	-5.3	0.2%	0.0%	19.1%	0.0%
2-ethylhexan-1-ol	203-234-3	104-76-7	104767	170	Reach_629	85	4.42	0.18	6	3.42	0.18		-3.9	-3.6	-4.7	0.0%	0.0%	19.1%	0.0%
2,4,6-trinitrotoluene	204-289-6	118-96-7	118967	349	Reach_975	86	3.58	0.58	25	3.13	0.78	10	-3.6	-3.6	-4.4	0.0%	0.0%	19.1%	0.0%
2-butoxyethanol	203-905-0	111-76-2	111762	309	Reach_869	87	6.10	0.25	8	5.10	0.25		-3.8	-3.6	-5.2	0.0%	0.0%	19.1%	0.0%
ethylene oxide	200-849-9	75-21-8	75218	854	Reach_134	88	5.17	0.70	28	4.17	0.70		-4.0	-3.7	-5.2	0.0%	0.0%	19.1%	0.0%
2,2-dimethylpropane-1,3-diol	204-781-0	126-30-7	126307	1805	Reach_1085	89	5.79	0.81	3				-3.0	-3.7	-5.3	0.1%	0.0%	19.2%	0.0%
nitrilotrimethylenetris(phosphonic acid)	229-146-5	6419-19-8	6419198	3429	Reach_2181	90	5.29	0.70	3	4.47	0.51		-2.8	-3.7	-5.2	0.3%	0.0%	19.2%	0.0%
sodium 2-hydroxyethanesulphonate	216-343-6	1562-00-1	1562001	5719	Reach_1692	91				5.00			-3.4	-3.7	-5.0	0.0%	0.0%	19.2%	0.0%
dichloro(dimethyl)silane	200-901-0	75-78-5	75785	3687	Reach_162	92	5.59	0.11	3	4.59	0.11		-4.0	-3.7	-5.6	0.0%	0.0%	19.2%	0.0%
2-(2-butoxyethoxy)ethanol	203-961-6	112-34-5	112345	326	Reach_899	93	6.25	0.70	32	5.20	0.70		-3.1	-3.7	-5.3	0.1%	0.0%	19.2%	0.0%
di(benzothiazol-2-yl) disulphide	204-424-9	120-78-5	120785	360	Reach_1001	94	4.50	0.70	3	4.60	0.75		-3.6	-3.7	-4.5	0.0%	0.0%	19.2%	0.0%
4-nitrophenol	202-811-7	100-02-7	100027	1	Reach_548	95	4.10	0.84	116	3.33	0.37		-3.4	-3.7	-4.5	0.0%	0.0%	19.2%	0.0%
1,5-naphthylenediamine	203-583-1	108-44-1	108441	239	Reach_745	96	4.03	1.02	5	2.02	1.19		-3.4	-3.7	-4.4	0.0%	0.0%	19.2%	0.0%
docusate sodium	209-406-4	577-11-7	577117	1224	Reach_1381	97	4.56	0.26	5	3.56	0.26		-3.4	-3.7	-5.0	0.0%	0.0%	19.2%	0.0%
pivalic acid	200-922-5	75-98-9	75989	868	Reach_168	98	5.60	0.64	4	4.60	0.64		-3.8	-3.7	-4.5	0.0%	0.0%	19.2%	0.0%
1-methyl-2-pyrrolidone	212-828-1	872-50-4	872504	977	Reach_1580	99	5.91	0.13	3	5.09	0.33		-3.6	-3.7	-5.1	0.0%	0.0%	19.3%	0.0%
propan-2-ol	200-661-7	67-63-0	67630	794	Reach_85	100	6.65	0.70	56	6.01	0.70		-3.9	-3.7	-4.7	0.0%	0.0%	19.3%	0.0%
(1-hydroxyethylidene)bisphosphonic acid, sodium salt	249-559-4	29329-71-3	29329713	5823	Reach_2629	101	5.51	1.50	3	4.51	1.50		-3.5	-3.7	-5.1	0.0%	0.0%	19.3%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [·]	Z(Cwfresh) [·]	Z(Cwcoast) [·]	TP(Cwlocal) [-]	TP(Cwfresh) [-]		TP(Cwcoast) [-]
benzoic acid	200-618-2	65-85-0	65850	785	Reach_77	102	4.96	0.66	12	3.50	0.70	20	-3.2	-3.7	-5.3	0.1%	0.0%	19.3%	0.0%
edetic acid	200-449-4	60-00-4	60004	71	Reach_53	103	4.92	0.69	7	3.92	0.69		-2.9	-3.7	-4.8	0.2%	0.0%	19.3%	0.0%
o-toluidine	202-429-0	95-53-4	95534	1032	Reach_432	104	4.63	0.80	11	2.93	1.37	3	-3.2	-3.7	-5.2	0.1%	0.0%	19.3%	0.0%
1-methylpyridinium chloride	662-772-0	25601-41-6	25601416	2440	Reach_4614	105	3.47	0.45	3	2.35	0.72		-3.5	-3.7	-5.1	0.0%	0.0%	19.3%	0.0%
toluene-4-sulphonic acid	203-180-0	104-15-4	104154	1385	Reach_619	106	5.62		2				-2.8	-3.7	-5.3	0.2%	0.0%	19.3%	0.0%
[[(phosphonomethyl)imino]bis[(ethylenenitrilo)bis(methylene)]]	244-751-4	22042-96-2	22042962	5777	Reach_2514	107	5.41	1.21	3	4.39	1.46		-3.5	-3.7	-5.1	0.0%	0.0%		0.0%
617-449-9	617-449-9	83196-58-1	83196581	3843	Reach_4463	108	3.06	0.17	3				-3.2	-3.7	-5.1	0.1%	0.0%		0.0%
buta-1,3-diene	203-450-8	106-99-0	106990	1453	Reach_688	109	4.46	0.23	3	3.46	0.23		-4.0	-3.7	-6.2	0.0%	0.0%		0.0%
methylammonium nitrate	244-787-0	22113-87-7	22113877	5779	Reach_2517	110	5.12		2				-3.5	-3.7	-5.1	0.0%	0.0%		0.0%
formaldehyde	200-001-8	50-00-0	50000	651	Reach_1	111	4.60	0.72	44	4.12	1.17	7	-4.0	-3.7	-5.1	0.0%	0.0%		0.0%
dimethyl phosphonate	212-783-8	868-85-9	868859	976	Reach_1575	112	5.05	0.42	4	4.03	0.49		-4.0	-3.7	-4.7	0.0%	0.0%		0.0%
resorcinol	203-585-2	108-46-3	108463	240	Reach_747	113	4.52	0.73	13	4.22	1.12	4	-3.4	-3.7	-4.8	0.0%	0.0%		0.0%
sodium p-cumenesulphonate	239-854-6	15763-76-5	15763765	5723	Reach_2396	114	5.50	0.70	3	4.50	0.70		-3.5	-3.7	-5.1	0.0%	0.0%		0.0%
tris(2-chloro-1-methylethyl) phosphate	237-158-7	13674-84-5	13674845	24	Reach_2342	115	4.81	0.29	12	3.81	0.29	12	-4.0	-3.7	-4.7	0.0%	0.0%		0.0%
3-chloro-p-toluidine	214-770-2	1193-21-1	1193211	1689	Reach_1670	116	3.52		2				-3.7	-3.7	-4.6	0.0%	0.0%		0.0%
toluene	203-625-9	108-88-3	108883	247	Reach_760	117	4.65	0.74	37	3.35	0.33	4	-4.0	-3.7	-5.8	0.0%	0.0%		0.0%
4,4'-methylenediphenyl diisocyanate	202-966-0	101-68-8	101688	1325	Reach_580	118	6.37	0.26	3	5.37	0.26		-3.9	-3.7	-5.2	0.0%	0.0%		0.0%
[2-(methacryloyloxy)ethyl]trimethylammonium chloride	225-733-5	5039-78-1	5039781	5898	Reach_2073	119	4.84	1.01	3	3.84	1.01		-3.5	-3.7	-5.1	0.0%	0.0%		0.0%
2-nitroaniline	260-480-4	56966-52-0	56966520	3219	Reach_2823	120	2.14		2				-4.0	-3.7	-4.5	0.0%	0.0%		0.0%
dodecane-12-lactam	213-424-8	947-04-6	947046	4110	Reach_1615	121	4.94	0.23	3	4.23	0.36		-3.6	-3.8	-5.2	0.0%	0.0%		0.0%
bis(2-propylheptyl) phthalate	258-469-4	53306-54-0	53306540	3094	Reach_2791	122	5.87	1.42	3	4.87	1.42		-3.8	-3.8	-4.2	0.0%	0.0%		0.0%
dimethyl sulphate	201-058-1	77-78-1	77781	886	Reach_185	123	4.24	0.26	5	3.43	0.16		-4.0	-3.8	-5.2	0.0%	0.0%		0.0%
chloromethane	200-817-4	74-87-3	74873	838	Reach_113	124	5.55	0.24	5	4.55	0.24		-4.2	-3.8	-5.8	0.0%	0.0%		0.0%
acetone	200-662-2	67-64-1	67641	795	Reach_86	125	6.60	0.86	49	4.69	2.42	7	-4.0	-3.8	-5.3	0.0%	0.0%		0.0%
sodium 2-sulphonatoethyl laurate	230-949-8	7381-01-3	7381013	5586	Reach_2244	126	4.78	1.29	3	3.78	1.29		-3.5	-3.8	-5.1	0.0%	0.0%		0.0%
naphthalene	202-049-5	91-20-3	91203	107	Reach_372	127	3.62	0.48	36	3.17	0.55	7	-4.0	-3.8	-4.8	0.0%	0.0%		0.0%
N-(carboxymethyl)-N-(phosphonomethyl)glycine	203-606-5	108-68-9	108689	243	Reach_752	128	4.21	0.84	20	3.21	0.84		-2.9	-3.8	-5.4	0.2%	0.0%		0.0%
cyclohexane	203-806-2	110-82-7	110827	285	Reach_830	129	4.80	0.99	13	3.80	0.70	52	-4.1	-3.8	-6.0	0.0%	0.0%		0.0%
isononyl alcohol	248-471-3	27458-94-2	27458942	2507	Reach_2605	130	3.99	0.17	3	3.26	0.20		-4.0	-3.8	-5.0	0.0%	0.0%		0.0%
formamide	200-842-0	75-12-7	75127	851	Reach_131	131	6.41	0.93	4	4.70	0.70		-3.5	-3.8	-5.4	0.0%	0.0%		0.0%
sodium 2-methyl-2-[(1-oxoallyl)amino]propanesulphonate	225-948-4	5165-97-9	5165979	5908	Reach_2082	132	6.60	0.17	3	5.60	0.17		-3.6	-3.8	-5.2	0.0%	0.0%		0.0%
potassium phenylacetate	201-155-9	78-90-0	78900	904	Reach_215	133	5.31	0.66	4	4.31	0.66		-3.6	-3.8	-5.2	0.0%	0.0%		0.0%
adiponitrile	203-896-3	111-69-3	111693	307	Reach_865	134	5.93	0.26	5	4.93	0.26		-3.5	-3.8	-5.4	0.0%	0.0%		0.0%
isobutane	200-857-2	75-28-5	75285	3661	Reach_136	135	4.42	0.38	3	3.42	0.38		-4.1	-3.8	-6.3	0.0%	0.0%		0.0%
2,6-xylenol	209-400-1	576-26-1	576261	723	Reach_1380	136	3.85	0.84	28	2.85	0.84		-4.1	-3.8	-4.8	0.0%	0.0%		0.0%
2,4-dichlorophenol	202-634-5	98-07-7	98077	1065	Reach_496	137	5.34	1.11	3	4.34	1.11		-4.1	-3.8	-4.6	0.0%	0.0%		0.0%
dimethyl sulfoxide	200-664-3	67-68-5	67685	796	Reach_88	138	7.53	0.52	14	6.53	0.70	56	-4.1	-3.8	-4.6	0.0%	0.0%		0.0%
nicotinonitrile	202-863-0	100-54-9	100549	131	Reach_563	139	5.63	0.23	3	4.63	0.23		-3.3	-3.8	-4.6	0.1%	0.0%		0.0%
2-(1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3	207-586-9	482-89-3	482893	647	Reach_1292	140	6.41	0.85	3	5.41	0.85		-3.5	-3.8	-4.6	0.0%	0.0%		0.0%
methenamine	202-905-8	100-97-0	100970	2	Reach_571	141	7.59	0.70	24	6.59	0.70		-3.0	-3.8	-5.4	0.1%	0.0%		0.0%
vinyl acetate	203-545-4	108-05-4	108054	228	Reach_727	142	4.61	0.56	10	3.61	0.56		-4.1	-3.8	-5.4	0.0%	0.0%		0.0%
diallyldimethylammonium chloride	230-993-8	7398-69-8	7398698	1234	Reach_2248	143	4.31	0.75	6	3.31	0.75		-3.6	-3.8	-5.2	0.0%	0.0%		0.0%
triethyl phosphate	201-114-5	78-40-0	78400	894	Reach_198	144	5.58	1.01	45	5.26	0.75		-4.0	-3.9	-4.8	0.0%	0.0%		0.0%
sodium 3,5,6-trichloropyridin-2-olate	202-764-2	99-54-7	99547	1087	Reach_529	145	3.56	0.70	20	2.63	0.70		-3.6	-3.9	-5.2	0.0%	0.0%		0.0%
anthracene	203-697-1	109-70-6	109706	262	Reach_786	146	5.01	0.42	5	4.01	0.42		-4.1	-3.9	-4.7	0.0%	0.0%		0.0%
2-piperazin-1-ylethylamine	205-411-0	140-31-8	140318	449	Reach_1149	147	5.67	0.69	4	4.36	0.81		-3.8	-3.9	-5.1	0.0%	0.0%		0.0%
4,4'-sulphonyldiphenol	201-250-5	80-09-1	80091	97	Reach_257	148	4.90		2	3.43			-3.4	-3.9	-4.7	0.0%	0.0%		0.0%
2-dimethylaminoethanol	203-542-8	108-01-0	108010	227	Reach_725	149	5.05	0.55	3	4.25	0.75		-4.1	-3.9	-5.4	0.0%	0.0%		0.0%
ethane	200-814-8	74-84-0	74840	3646	Reach_110	150	4.42	0.38	3	3.42	0.38		-4.2	-3.9	-6.1	0.0%	0.0%		0.0%
1-chloro-4-nitrobenzene	203-397-0	106-43-4	106434	190	Reach_666	151	3.86	0.70	16	3.14	0.45		-4.1	-3.9	-4.8	0.0%	0.0%		0.0%
isophthalic acid	204-506-4	121-91-5	121915	1739	Reach_1022	152	5.35	0.87	3	4.35	0.87		-3.2	-3.9	-5.5	0.1%	0.0%		0.0%
bis(2-ethylhexyl) phthalate	204-211-0	117-81-7	117817	346	Reach_961	153	3.63	1.28	30	2.41	1.03	5	-3.8	-3.9	-4.9	0.0%	0.0%		0.0%
butan-1-ol	200-751-6	71-36-3	71363	819	Reach_101	154	6.11	0.70	40	5.17	0.70		-4.1	-3.9	-5.3	0.0%	0.0%		0.0%
potassium methanolate	212-736-1	865-33-8	865338	6064	Reach_1568	155	6.82	0.70	3	5.17	1.57		-3.7	-3.9	-5.2	0.0%	0.0%		0.0%
troclosene sodium	220-767-7	2893-78-9	2893789	1213	Reach_1880	156	3.44	1.42	6	2.55	1.78		-3.7	-3.9	-5.3	0.0%	0.0%		0.0%
guanidinium nitrate	208-060-1	506-93-4	506934	5900	Reach_1313	157	5.12	0.97	3	4.12	0.97		-3.7	-3.9	-5.3	0.0%	0.0%		0.0%
tris(2-hydroxyethyl)ammonium acetate	238-874-2	14806-72-5	14806725	5702	Reach_2369	158	5.40	0.27	3	4.40	0.27		-3.7	-3.9	-5.3	0.0%	0.0%		0.0%
methane	200-812-7	74-82-8	74828	3645	Reach_108	159	4.42	0.38	3	3.42	0.38		-4.5	-3.9	-6.1	0.0%	0.0%		0.0%
tris(2,4-ditert-butylphenyl) phosphite	250-709-6	31570-04-4	31570044	2629	Reach_2655	160	5.54	0.16	3	4.54	0.16		-4.1	-3.9	-2.3	0.0%	0.0%		1.2%
2-methoxy-2-methylbutane	213-611-4	994-05-8	994058	4205	Reach_1628	161	5.33	0.58	3	4.33	0.58		-4.2	-3.9	-5.4	0.0%	0.0%		0.0%
disodium 4,4'-bis[6-anilino-[4-[bis(2-hydroxyethyl)amino]-1,3,5-t	224-073-5	4193-55-9	4193559	5882	Reach_2020	162	5.39	0.64	3	4.39	0.64		-3.7	-3.9	-5.3	0.0%	0.0%		0.0%
sulphanilic acid	204-482-5	121-57-3	121573	372	Reach_1016	163	4.69	0.29	3	3.72	0.58		-3.3	-3.9	-4.8	0.0%	0.0%		0.0%

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Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
2-hydroxybenzimidazole	204-428-0	120-82-1	120821	362	Reach_1003	164	3.47	0.51	33	2.37	0.57	9	-3.3	-3.9	-5.5	0.1%	0.0%	0.0%
formic acid	200-579-1	64-18-6	64186	777	Reach_71	165	5.75	0.59	6	4.75	0.59		-2.9	-3.9	-5.6	0.2%	0.0%	0.0%
methyl methacrylate	201-297-1	80-62-6	80626	938	Reach_268	166	5.53	0.30	9	4.55	0.39		-4.2	-4.0	-5.2	0.0%	0.0%	0.0%
trichloro(methyl)silane	200-902-6	75-79-6	75796	3689	Reach_163	167	7.27	0.86	3	4.97	0.86		-4.3	-4.0	-5.7	0.0%	0.0%	0.0%
1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triaz	253-575-7	37640-57-6	37640576	5868	Reach_2711	168	6.19	0.64	3	5.27	0.84		-3.7	-4.0	-5.3	0.0%	0.0%	0.0%
2-pyrrolidone	210-483-1	616-45-5	616455	757	Reach_1432	169	6.07	1.17	3	5.07	1.17		-3.6	-4.0	-5.3	0.0%	0.0%	0.0%
trimethyl-3-[(1-oxoallyl)amino]propylammonium chloride	256-181-3	45021-77-0	45021770	5890	Reach_2757	170	5.29	0.34	3	4.29	0.34		-3.7	-4.0	-5.3	0.0%	0.0%	0.0%
4-chloro-o-cresol	216-381-3	1570-64-5	1570645	495	Reach_1696	171	3.46	0.84	24	2.46	0.84		-4.2	-4.0	-4.9	0.0%	0.0%	0.0%
thiram (reach)	205-286-2	137-26-8	137268	441	Reach_1137	172	2.18	1.10	36	1.11	1.00	7	-3.5	-4.0	-4.9	0.0%	0.0%	0.0%
3-dimethylaminopropiononitrile	217-090-4	1738-25-6	1738256	2132	Reach_1714	173	5.63	0.51	3	4.63	0.51		-4.1	-4.0	-5.6	0.0%	0.0%	0.0%
2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-N-p	228-787-8	6358-85-6	6358856	3410	Reach_2171	174	5.26	1.21	3	4.26	1.21		-3.8	-4.0	-5.5	0.0%	0.0%	0.0%
2,3,6-trimethylphenol	219-330-3	2416-94-6	2416946	558	Reach_1801	175	4.04	0.84	20	3.36	0.84		-4.2	-4.0	-4.9	0.0%	0.0%	0.0%
sodium [2-[(2,6-dichlorophenyl)amino]phenyl]acetate	239-346-4	15307-79-6	15307796	30	Reach_2381	176	4.53	0.64	11	3.45	1.51	6	-3.3	-4.0	-4.8	0.0%	0.0%	0.0%
potassium (R)-(4-hydroxyphenyl)[(3-methoxy-1-methyl-3-oxoprc	273-992-8	69416-61-1	69416611	6001	Reach_2915	177							-3.8	-4.0	-5.4	0.0%	0.0%	0.0%
butyl acrylate	205-480-7	141-32-2	141322	455	Reach_1161	178	3.74	0.49	4	2.83	0.46		-4.3	-4.0	-5.4	0.0%	0.0%	0.0%
sodium feredetate	239-802-2	15708-41-5	15708415	1199	Reach_2394	179	4.93	0.48	10	3.93	0.48		-3.8	-4.0	-5.4	0.0%	0.0%	0.0%
2-chloroethanol	203-459-7	107-07-3	107073	207	Reach_692	180	4.88	0.63	19	2.87	0.74	5	-4.2	-4.0	-5.4	0.0%	0.0%	0.0%
phthalonitrile	202-044-8	91-15-6	91156	1004	Reach_369	181	4.83	0.46	4	3.83	0.46		-4.1	-4.0	-5.1	0.0%	0.0%	0.0%
potassium (E,E)-hexa-2,4-dienoate	202-854-1	100-46-9	100469	127	Reach_559	182	4.79	0.29	4	3.90	0.27		-3.8	-4.0	-5.4	0.0%	0.0%	0.0%
o-phenylenediamine	202-430-6	95-54-5	95545	1033	Reach_433	183	3.84	0.90	4	2.84	0.90		-3.6	-4.0	-4.8	0.0%	0.0%	0.0%
3-aminomethyl-3,5,5-trimethylcyclohexylamine	220-666-8	2855-13-2	2855132	2536	Reach_1875	184	4.86	0.57	3	3.74	0.59		-4.1	-4.0	-5.6	0.0%	0.0%	0.0%
acetic anhydride	203-564-8	108-24-7	108247	234	Reach_737	185	5.45	0.94	4	5.27	0.92		-4.2	-4.0	-5.4	0.0%	0.0%	0.0%
1-nitroguanidine	209-143-5	556-88-7	556887	707	Reach_1370	186	5.92	0.87	7	5.09	1.10		-3.1	-4.0	-5.6	0.1%	0.0%	0.0%
3-methylpyridine	203-636-9	108-99-6	108996	253	Reach_767	187	5.58	0.30	5	4.58	0.30		-3.8	-4.0	-4.9	0.0%	0.0%	0.0%
benzyl(methyl)amine	203-133-4	103-67-3	103673	1376	Reach_610	188	3.87	0.78	3				-4.3	-4.0	-5.2	0.0%	0.0%	0.0%
2-(2-methoxyethoxy)ethanol	203-906-6	111-77-3	111773	310	Reach_870	189	6.55	0.57	6	5.70	0.70		-3.7	-4.1	-5.7	0.0%	0.0%	0.0%
pyridine	203-809-9	110-86-1	110861	287	Reach_833	190	5.21	0.86	34	4.21	0.86	34	-3.6	-4.1	-5.7	0.0%	0.0%	0.0%
anthraquinone	201-549-0	84-65-1	84651	960	Reach_287	191	4.38	0.44	4	1.41	0.42		-3.9	-4.1	-4.9	0.0%	0.0%	0.0%
sodium sarcosinate	224-338-5	4316-73-8	4316738	5885	Reach_2027	192	6.25	1.09	3	5.25	1.09		-3.8	-4.1	-5.4	0.0%	0.0%	0.0%
o-xylene	202-422-2	95-47-6	95476	1028	Reach_428	193	4.04	0.62	26	3.04	0.70	104	-4.3	-4.1	-6.0	0.0%	0.0%	0.0%
2,3-epoxypropyltrimethylammonium chloride	221-221-0	3033-77-0	3033770	1214	Reach_1901	194	5.40	1.03	7	4.40	1.03		-3.8	-4.1	-5.4	0.0%	0.0%	0.0%
2-furaldehyde	202-627-7	98-01-1	98011	1064	Reach_495	195	4.31	0.31	13	3.04	0.82	5	-4.3	-4.1	-5.3	0.0%	0.0%	0.0%
2-(2-(2-methoxyethoxy)ethoxy)ethanol	203-962-1	112-35-6	112356	1584	Reach_900	196	7.50	0.74	3	6.50	0.74		-3.3	-4.1	-5.8	0.0%	0.0%	0.0%
2-methylpropene	204-066-3	115-11-7	115117	1631	Reach_937	197	4.13	0.25	3	3.13	0.25		-4.3	-4.1	-6.7	0.0%	0.0%	0.0%
2,2'-ethylenedioxydiethyl bis(2-ethylhexanoate)	202-319-2	94-28-0	94280	4100	Reach_413	198	4.59		1				-4.1	-4.1	-5.4	0.0%	0.0%	0.0%
N-(1-cyanoethyl)formamide	248-440-4	27394-99-6	27394996	2503	Reach_2604	199	5.83		1				-3.4	-4.1	-5.7	0.0%	0.0%	0.0%
2,6-xylidine	201-758-7	87-62-7	87627	980	Reach_314	200	4.90	0.31	5	3.90	0.31		-3.9	-4.1	-5.2	0.0%	0.0%	0.0%
2,2'-(ethylenedioxy)diethanol	203-953-2	112-27-6	112276	322	Reach_894	201	7.08	0.73	12	6.08	0.70	48	-3.2	-4.1	-5.8	0.1%	0.0%	0.0%
tris[2-chloro-1-(chloromethyl)ethyl] phosphate	237-159-2	13674-87-8	13674878	25	Reach_2343	202	3.65	0.44	8	2.67	0.34		-4.2	-4.1	-5.0	0.0%	0.0%	0.0%
carbazole	201-696-0	86-74-8	86748	974	Reach_303	203	3.78	0.72	6	2.78	0.70		-4.0	-4.1	-4.9	0.0%	0.0%	0.0%
3,5,5-trimethylcyclohex-2-enone	201-126-0	78-59-1	78591	897	Reach_201	204	5.31	0.70	40	4.71	0.39		-4.3	-4.1	-5.1	0.0%	0.0%	0.0%
cyanamide (reach)	206-992-3	420-04-2	420042	636	Reach_1268	205	3.96	0.73	12	2.99	0.86	5	-3.5	-4.1	-4.9	0.0%	0.0%	0.0%
(17α)-17-hydroxy-3-oxoandrost-4-ene-17-carbonitrile	278-780-9	77881-13-1	77881131	3742	Reach_2952	206	3.01	0.17	3				-3.4	-4.1	-5.6	0.0%	0.0%	0.0%
undec-10-enoic acid	203-965-8	112-38-9	112389	1585	Reach_902	207	4.07	0.79	3	3.21	0.76		-4.3	-4.1	-5.6	0.0%	0.0%	0.0%
methyl acetate	201-185-2	79-20-9	79209	916	Reach_234	208	5.67	0.21	3	4.85	0.21		-4.3	-4.1	-5.2	0.0%	0.0%	0.0%
1-chloro-2,3-epoxypropane	203-439-8	106-89-8	106898	200	Reach_680	209	4.32	0.68	18	3.32	0.68		-4.3	-4.1	-5.2	0.0%	0.0%	0.0%
disodium 4,4'-diaminostilbene-2,2'-disulphonate	230-847-3	7336-20-1	7336201	6014	Reach_2239	210	5.47		1				-3.9	-4.1	-5.5	0.0%	0.0%	0.0%
3,3'-dichlorobenzidine dihydrochloride	210-323-0	612-83-9	612839	5949	Reach_1422	211	3.53	0.31	3	2.54	0.39		-3.9	-4.1	-5.5	0.0%	0.0%	0.0%
4-hydroxy-4-methylpentan-2-one	204-626-7	123-42-2	123422	393	Reach_1050	212	6.48	0.56	6	5.48	0.56		-4.3	-4.1	-5.7	0.0%	0.0%	0.0%
N-tert-butylbenzothiazole-2-sulphenamide	202-409-1	95-31-8	95318	4124	Reach_425	213	2.72	0.46	3	1.93	0.76		-4.3	-4.1	-5.6	0.0%	0.0%	0.0%
1-vinyl-2-pyrrolidone	201-800-4	88-12-0	88120	3948	Reach_316	214	5.48	1.07	3	4.48	1.07		-4.1	-4.1	-5.8	0.0%	0.0%	0.0%
octadecan-1-ol	204-017-6	112-92-5	112925	1611	Reach_930	215	5.19	1.82	3	4.19	1.82		-4.0	-4.1	-5.1	0.0%	0.0%	0.0%
3-aminophenol	209-711-2	591-27-5	591275	734	Reach_1391	216	4.09	1.00	4	3.09	0.84		-3.8	-4.1	-4.9	0.0%	0.0%	0.0%
p-toluidine	203-403-1	106-49-0	106490	195	Reach_671	217	4.57	1.03	6	2.53	1.35		-3.6	-4.1	-5.7	0.0%	0.0%	0.0%
benzothiazole	202-396-2	95-16-9	95169	113	Reach_423	218	4.58	0.58	10	3.75	0.51		-3.8	-4.1	-4.9	0.0%	0.0%	0.0%
tetrasodium N,N-bis(carboxylatomethyl)-L-glutamate	257-573-7	51981-21-6	51981216	5910	Reach_2777	219	6.10	0.38	3	5.10	0.38		-3.9	-4.1	-5.5	0.0%	0.0%	0.0%
1,3,5-triazine-2,4,6(1H,3H,5H)-trione, trisodium salt	221-255-6	3047-33-4	3047334	5834	Reach_1905	220	6.61	0.46	3	5.61	0.46		-3.9	-4.1	-5.5	0.0%	0.0%	0.0%
butan-2-ol	201-158-5	78-92-2	78922	905	Reach_216	221	6.39	0.26	7	5.39	0.26		-4.3	-4.1	-5.2	0.0%	0.0%	0.0%
sebacic acid	203-845-5	111-20-6	111206	1541	Reach_848	222	4.42		2				-3.6	-4.1	-5.8	0.0%	0.0%	0.0%
2-hydroxyethyl methacrylate	212-782-2	868-77-9	868779	975	Reach_1574	223	5.31	0.39	5	4.88	0.23		-4.3	-4.1	-5.7	0.0%	0.0%	0.0%
[(methylethylene)bis(oxy)]dipropanol	246-466-0	24800-44-0	24800440	2404	Reach_2555	224	6.74	0.60	3	5.74	0.60		-3.6	-4.1	-5.7	0.0%	0.0%	0.0%
1-aminopropan-2-ol	201-162-7	78-96-6	78966	907	Reach_219	225	5.44	0.64	6	4.44	0.64		-4.3	-4.2	-5.6	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [·]	Z(Cwfresh) [·]	Z(Cwcoast) [·]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
pyrithione zinc	236-671-3	13463-41-7	13463417	1190	Reach_2336	226	1.49	1.53	24	0.81	1.02	10	-3.9	-4.2	-5.5	0.0%	0.0%	0.0%
hexamethylene diisocyanate	212-485-8	822-06-0	822060	3822	Reach_1555	227	5.06	0.43	3	4.06	0.43		-4.4	-4.2	-5.6	0.0%	0.0%	0.0%
2-hydroxy-4-(methylthio)butyronitrile	241-756-3	17773-41-0	17773410	2152	Reach_2443	228	3.03		1				-3.8	-4.2	-5.8	0.0%	0.0%	0.0%
sodium hydroxymethanesulphinate	205-739-4	149-44-0	149440	5704	Reach_1199	229	5.09	0.36	3	4.09	0.36		-3.9	-4.2	-5.5	0.0%	0.0%	0.0%
2-methylglutaronitrile	253-506-0	37439-34-2	37439342	5867	Reach_2710	230	4.18		2				-3.8	-4.2	-5.7	0.0%	0.0%	0.0%
sodium dodecyl sulphate	205-788-1	151-21-3	151213	1198	Reach_1207	231	3.74	0.60	80	2.94	0.52	13	-3.9	-4.2	-5.5	0.0%	0.0%	0.0%
3,5-dichloroaniline	210-948-9	626-43-7	626437	768	Reach_1457	232	3.62	0.84	20	2.62	0.84		-3.6	-4.2	-4.9	0.0%	0.0%	0.0%
pyrazole	224-923-5	4553-62-2	4553622	2942	Reach_2047	233	5.91		2				-3.4	-4.2	-5.7	0.0%	0.0%	0.0%
dichloro(methyl)silane	200-877-1	75-54-7	75547	3675	Reach_149	234	5.58		3	4.58			-4.5	-4.2	-6.0	0.0%	0.0%	0.0%
butanone	201-159-0	78-93-3	78933	906	Reach_217	235	6.35	0.40	9	5.35	0.40		-4.4	-4.2	-5.3	0.0%	0.0%	0.0%
N-(4-aminophenyl)aniline	202-951-9	101-54-2	101542	1323	Reach_579	236	3.09	0.46	3	2.42	0.55		-3.6	-4.2	-5.7	0.0%	0.0%	0.0%
sodium hydrogen glutamate	205-538-1	142-47-2	142472	5695	Reach_1178	237	4.69	1.35	3	3.69	1.35		-3.9	-4.2	-5.5	0.0%	0.0%	0.0%
benzyl alcohol	202-859-9	100-51-6	100516	129	Reach_561	238	5.09	0.64	14	4.21	0.50	3	-4.4	-4.2	-5.7	0.0%	0.0%	0.0%
butyraldehyde	204-646-6	123-72-8	123728	396	Reach_1056	239	5.12	0.63	5	4.39	0.29		-4.4	-4.2	-5.6	0.0%	0.0%	0.0%
2-chloropyridine	203-646-3	109-09-1	109091	255	Reach_770	240	4.53	1.69	4	3.53	1.69		-3.5	-4.2	-4.9	0.0%	0.0%	0.0%
dimethylammonium 2,4-dichlorophenoxyacetate	217-915-8	2008-39-1	2008391	1202	Reach_1744	241	5.18	0.84	56	4.13	1.04		-3.9	-4.2	-5.5	0.0%	0.0%	0.0%
C,C'-azodi(formamide)	204-650-8	123-77-3	123773	1775	Reach_1058	242	4.63	0.37	3	3.63	0.37		-3.4	-4.2	-5.9	0.0%	0.0%	0.0%
tetrasodium (1-hydroxyethylidene)bisphosphonate	223-267-7	3794-83-0	3794830	5869	Reach_1992	243	5.26	1.48	3	4.26	1.48		-3.9	-4.2	-5.5	0.0%	0.0%	0.0%
tetrahydrothiophene 1,1-dioxide	204-783-1	126-33-0	126330	406	Reach_1086	244	5.79	0.56	4	4.79	0.56		-4.1	-4.2	-5.0	0.0%	0.0%	0.0%
2,4,6-tribromophenol	204-278-6	118-79-6	118796	348	Reach_970	245	3.30	0.59	5	2.24	0.84		-4.4	-4.2	-5.1	0.0%	0.0%	0.0%
1,4-diazabicyclooctane	205-999-9	280-57-9	280579	577	Reach_1219	246	5.70	0.61	3	4.61	0.49		-4.1	-4.2	-5.0	0.0%	0.0%	0.0%
3,5-xylenol	204-680-1	124-10-7	124107	1784	Reach_1068	247	6.23		1				-4.4	-4.2	-5.6	0.0%	0.0%	0.0%
dodecan-1-ol	203-982-0	112-53-8	112538	332	Reach_911	248	3.02	0.61	6	2.02	0.61		-4.4	-4.2	-5.5	0.0%	0.0%	0.0%
2,5-dichloroaniline	202-455-2	95-82-9	95829	1040	Reach_444	249	3.56	0.73	9	2.56	0.73		-3.6	-4.2	-5.0	0.0%	0.0%	0.0%
ethyl acetate	205-500-4	141-78-6	141786	458	Reach_1168	250	5.80	0.45	29	4.08	0.87	3	-4.4	-4.2	-5.6	0.0%	0.0%	0.0%
dimethylamine	204-697-4	124-40-3	124403	17	Reach_1077	251	4.89	0.52	11	3.67	0.45	3	-4.5	-4.2	-5.3	0.0%	0.0%	0.0%
2-methylbutane	201-142-8	78-78-4	78784	3758	Reach_208	252	3.98	0.50	3	2.98	0.50		-4.5	-4.2	-6.7	0.0%	0.0%	0.0%
cyanoguanidine	207-312-8	461-58-5	461585	2948	Reach_1283	253	6.56	0.82	3	5.56	0.82		-3.3	-4.2	-5.8	0.1%	0.0%	0.0%
p-cresol	203-398-6	106-44-5	106445	191	Reach_667	254	4.09	0.84	48	3.38	0.77		-4.4	-4.2	-5.7	0.0%	0.0%	0.0%
1,1',1''-nitrilotripropan-2-ol	204-528-4	122-20-3	122203	1743	Reach_1027	255	5.86	0.72	3	4.68	1.17		-3.4	-4.2	-5.9	0.0%	0.0%	0.0%
[3-methyl-5-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4-pentadienyl]	212-028-2	751-83-7	751837	6024	Reach_1525	256	1.78		1				-3.9	-4.2	-5.6	0.0%	0.0%	0.0%
(4-chlorophenyl)hydrazine	202-446-3	95-74-9	95749	1037	Reach_439	257	3.98	0.63	11	2.98	0.63	11	-3.7	-4.2	-5.7	0.0%	0.0%	0.0%
2-hydroxyethyl acrylate	212-454-9	818-61-1	818611	943	Reach_1552	258	3.73	0.34	4	2.86	0.56		-4.3	-4.2	-5.8	0.0%	0.0%	0.0%
2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-din	225-822-9	5102-83-0	5102830	3025	Reach_2078	259	5.26	1.21	3	4.26	1.21		-3.9	-4.2	-5.8	0.0%	0.0%	0.0%
tris(2-ethylhexyl) benzene-1,2,4-tricarboxylate	222-020-0	3319-31-1	3319311	2676	Reach_1945	260	-0.55	1.62	3	3.33			-4.4	-4.2	-4.7	0.0%	0.0%	0.0%
p-cumenesulphonic acid	240-210-1	16066-35-6	16066356	2076	Reach_2410	261	5.62		2				-3.4	-4.2	-5.8	0.0%	0.0%	0.0%
sodium hydrogen 4-amino-5-hydroxynaphthalene-2,7-disulphon	226-736-4	5460-09-3	5460093	5583	Reach_2116	262	5.94		1				-4.0	-4.2	-5.6	0.0%	0.0%	0.0%
tetradecanol	204-000-3	112-72-1	112721	1599	Reach_920	263	2.60	0.47	3	1.60	0.47		-4.4	-4.2	-5.4	0.0%	0.0%	0.0%
4-methyl-m-phenylenediamine	202-453-1	95-80-7	95807	1039	Reach_443	264	4.95	1.44	5	3.95	1.44		-3.7	-4.2	-5.0	0.0%	0.0%	0.0%
2-methylpentane-2,4-diol	203-489-0	107-41-5	107415	219	Reach_706	265	6.91	0.22	19	5.91	0.22	19	-4.1	-4.2	-5.7	0.0%	0.0%	0.0%
4-tert-butylbenzoic acid	202-696-3	98-73-7	98737	1075	Reach_517	266	4.43	0.69	3	3.43	0.69		-4.2	-4.2	-5.1	0.0%	0.0%	0.0%
2-(2-ethoxyethoxy)ethanol	203-919-7	111-90-0	111900	315	Reach_880	267	7.11	0.31	14	6.11	0.31	14	-3.8	-4.2	-5.9	0.0%	0.0%	0.0%
4-chlorophenol	203-402-6	106-48-9	106489	194	Reach_670	268	3.98	0.84	88	2.69	0.32		-4.5	-4.2	-5.0	0.0%	0.0%	0.0%
4-(1,1,3,3-tetramethylbutyl)phenol	205-426-2	140-66-9	140669	451	Reach_1150	269	2.32	0.71	8	1.74	0.51		-4.3	-4.2	-5.1	0.0%	0.0%	0.0%
L-menthol	218-690-9	2216-51-5	2216515	538	Reach_1773	270	4.32	0.13	4	3.66	0.16		-4.4	-4.2	-5.6	0.0%	0.0%	0.0%
diclofenac	239-348-5	15307-86-5	15307865	31	Reach_2382	271	4.31	0.63	17	1.93	1.50	14	-4.1	-4.2	-5.0	0.0%	0.0%	0.0%
disodium dihydrogen ethylenediaminetetraacetate	205-358-3	139-33-3	139333	5686	Reach_1143	272	4.84	0.78	3	4.51	1.00		-4.0	-4.2	-5.6	0.0%	0.0%	0.0%
N,N''-(isobutylidene)diurea	228-055-8	6104-30-9	6104309	3324	Reach_2153	273	5.70		1				-4.1	-4.3	-6.0	0.0%	0.0%	0.0%
1,3-dimethylurea	202-498-7	96-31-1	96311	1052	Reach_460	274	6.61	0.66	4	5.61	0.66		-3.8	-4.3	-5.1	0.0%	0.0%	0.0%
[[(phosphonomethyl)imino]bis[ethane-2,1-diylnitrilobis(methyle	239-931-4	15827-60-8	15827608	2059	Reach_2401	275	4.97	1.40	3	3.97	1.40		-3.4	-4.3	-5.8	0.0%	0.0%	0.0%
m-phenylenebis(methylamine)	216-032-5	1477-55-0	1477550	1997	Reach_1686	276	4.52	0.29	3	3.84	0.38		-4.5	-4.3	-5.7	0.0%	0.0%	0.0%
O-benzyl-L-valine toluene-p-sulphonate	240-702-6	16652-76-9	16652769	5735	Reach_2425	277	4.86		2	4.51			-4.0	-4.3	-5.6	0.0%	0.0%	0.0%
N-methylaniline	253-657-2	37763-23-8	37763238	2807	Reach_2712	278	3.90	0.59	3				-4.5	-4.3	-5.0	0.0%	0.0%	0.0%
disodium 4,4'-bis[(4-anilino-6-morpholino-1,3,5-triazin-2-yl)amin	240-245-2	16090-02-1	16090021	1200	Reach_2412	279	5.41	0.82	4	4.41	0.82		-4.0	-4.3	-5.6	0.0%	0.0%	0.0%
tris(nonylphenyl) phosphite	247-759-6	26523-78-4	26523784	2474	Reach_2585	280	4.12	1.37	3	3.12	1.37		-4.5	-4.3	-1.8	0.0%	0.0%	3.3%
o-cresol	202-423-8	95-48-7	95487	1029	Reach_429	281	4.48	0.84	144	3.40	0.45		-4.5	-4.3	-5.7	0.0%	0.0%	0.0%
potassium hydrogen oxalate	204-873-0	127-95-7	127957	5652	Reach_1103	282	5.80	0.68	3	4.80	0.68		-4.0	-4.3	-5.6	0.0%	0.0%	0.0%
bis(pentane-2,4-dionato)calcium	243-001-3	19372-44-2	19372442	5757	Reach_2477	283	4.71	0.48	3	3.71	0.48		-4.0	-4.3	-5.6	0.0%	0.0%	0.0%
2,4,5-trichloroaniline	211-254-9	636-30-6	636306	774	Reach_1474	284	3.46	0.84	12	2.46	0.84		-3.9	-4.3	-5.0	0.0%	0.0%	0.0%
1,1'-iminodipropan-2-ol	203-820-9	110-97-4	110974	292	Reach_840	285	5.69	0.47	5	4.91	0.34		-3.7	-4.3	-5.7	0.0%	0.0%	0.0%
potassium 2-ethylhexanoate	221-625-7	3164-85-0	3164850	5842	Reach_1924	286	5.14	0.45	3	4.27	0.37		-4.0	-4.3	-5.6	0.0%	0.0%	0.0%
2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-chlor	226-939-8	5567-15-7	5567157	706	Reach_2124	287	4.56	0.35	4	4.26	1.21		-4.1	-4.3	-5.6	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
bis(pentabromophenyl) ether	214-604-9	1163-19-5	1163195	345	Reach_1664	288	-1.49	0.92	3							0.0%	0.0%	0.0%
6-aminopenicillanic acid	208-993-4	551-16-6	551166	3161	Reach_1357	289	4.63		1				-3.4	-4.3	-5.8	0.0%	0.0%	0.0%
2-(2-pyridyl)ethanol	203-140-2	103-74-2	103742	163	Reach_614	290	5.38	1.11	4	4.38	1.11		-3.8	-4.3	-5.3	0.0%	0.0%	0.0%
dichloromethane	200-838-9	75-09-2	75092	850	Reach_129	291	5.40	0.57	17	5.33	0.49	3	-4.6	-4.3	-6.2	0.0%	0.0%	0.0%
17β-hydroxy-17-(3-hydroxy-1-propynyl)androst-4-ene-3-one	259-700-1	55542-26-2	55542262	3172	Reach_2807	292	4.72		2				-3.6	-4.3	-5.8	0.0%	0.0%	0.0%
pentane	203-692-4	109-66-0	109660	260	Reach_783	293	3.86	0.54	3	2.86	0.70		-4.5	-4.3	-6.8	0.0%	0.0%	0.0%
3-chloropropane-1,2-diol	202-492-4	96-24-2	96242	1050	Reach_457	294	6.60	0.25	3	5.60	0.25		-3.7	-4.3	-5.9	0.0%	0.0%	0.0%
1-naphthylamine	700-846-7	274693-53-7	274693537	2508	Reach_5010	295	4.26	0.75	3				-4.0	-4.3	-5.1	0.0%	0.0%	0.0%
1-chloro-2-nitrobenzene	201-854-9	88-73-3	88733	986	Reach_330	296	4.20	0.70	24	3.41	0.53		-4.5	-4.3	-5.3	0.0%	0.0%	0.0%
tetrakis(hydroxymethyl)phosphonium chloride	204-707-7	124-64-1	124641	5637	Reach_1080	297	3.03	2.08	3	2.67	1.29		-4.0	-4.3	-5.6	0.0%	0.0%	0.0%
methacrylic acid	201-204-4	79-41-4	79414	3776	Reach_245	298	4.97	0.67	3	4.03	0.64		-3.8	-4.3	-5.9	0.0%	0.0%	0.0%
11-aminoundecanoic acid	219-417-6	2432-99-7	2432997	2387	Reach_1808	299	4.54		1				-3.4	-4.3	-6.0	0.0%	0.0%	0.0%
methoxyammonium chloride	604-045-2	137862-53-4	137862534	442	PharmaBeta_775	300	5.15	0.55	3	4.15	0.55		-4.1	-4.3	-5.6	0.0%	0.0%	0.0%
3,5,7-triaza-1-azoniatricyclo[3.3.1.13,7]decane nitrate	687-538-5	18423-20-6	18423206	5747	Reach_4635	301	4.64		1				-4.0	-4.3	-5.6	0.0%	0.0%	0.0%
tris(2-butoxyethyl) phosphate	201-122-9	78-51-3	78513	93	Reach_200	302	4.50	0.33	7	3.64	0.28		-4.5	-4.3	-5.3	0.0%	0.0%	0.0%
tributyl phosphate	204-800-2	126-73-8	126738	19	Reach_1089	303	4.10	1.01	78	3.56	0.40		-4.5	-4.3	-5.3	0.0%	0.0%	0.0%
propylenediamine	235-845-6	13005-36-2	13005362	5655	Reach_2316	304							-4.5	-4.3	-5.5	0.0%	0.0%	0.0%
1,2-dichloro-3-nitrobenzene	221-717-7	3209-22-1	3209221	600	Reach_1932	305	3.54	0.70	20	2.54	0.70		-4.5	-4.3	-5.3	0.0%	0.0%	0.0%
phthalimide	201-603-3	85-41-6	85416	965	Reach_294	306	4.36	0.45	4	3.64	0.91		-3.7	-4.3	-5.8	0.0%	0.0%	0.0%
tripotassium citrate	212-755-5	866-84-2	866842	6068	Reach_1571	307	6.34	0.43	3	5.34	0.43		-4.1	-4.3	-5.7	0.0%	0.0%	0.0%
2,2,6,6-tetramethylpiperidin-4-ol	219-291-2	2403-88-5	2403885	2368	Reach_1797	308	5.27	0.27	3	4.34	0.54		-4.5	-4.3	-5.9	0.0%	0.0%	0.0%
dinoseb	201-861-7	88-85-7	88857	989	Reach_333	309	2.55	0.64	16	2.01	1.36	5	-4.2	-4.3	-5.2	0.0%	0.0%	0.0%
benzophenone	204-337-6	119-61-9	119619	354	Reach_982	310	3.55	0.54	6	2.93	0.52		-4.5	-4.3	-5.2	0.0%	0.0%	0.0%
disodium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4-)-N,	239-407-5	15375-84-5	15375845	5714	Reach_2386	311	5.53	0.73	3	4.53	0.73		-4.1	-4.3	-5.7	0.0%	0.0%	0.0%
tetrasodium 4-amino-5-hydroxy-3,6-bis[[4-[[2-(sulphonatooxy)et	241-164-5	17095-24-8	17095248	5738	Reach_2430	312	4.95	0.68	3	3.88	0.91		-4.1	-4.3	-5.7	0.0%	0.0%	0.0%
atrazine (reach)	217-617-8	1912-24-9	1912249	37	Reach_1734	313	3.28	1.13	134	1.95	0.98	95	-4.1	-4.3	-5.1	0.0%	0.0%	0.0%
phenylhydrazine	202-873-5	100-63-0	100630	134	Reach_565	314	3.48	0.48	3	2.48	0.48		-4.2	-4.3	-5.4	0.0%	0.0%	0.0%
chloroform	200-663-8	67-66-3	67663	83	Reach_87	315	4.84	0.58	21	4.54	1.04	8	-4.7	-4.3	-6.3	0.0%	0.0%	0.0%
dimethyl phthalate	205-011-6	131-11-3	131113	417	Reach_1119	316	4.99	0.72	60	4.08	0.16		-4.5	-4.3	-5.9	0.0%	0.0%	0.0%
propionic acid	201-176-3	79-09-4	79094	913	Reach_229	317	4.97	0.37	7	3.97	0.37		-3.9	-4.3	-5.9	0.0%	0.0%	0.0%
benzothiazole-2-thiol	205-736-8	149-30-4	149304	478	Reach_1198	318	3.55	0.76	4	3.14	0.96		-4.4	-4.3	-5.1	0.0%	0.0%	0.0%
ibuprofen	258-868-3	53928-30-6	53928306	3115	Reach_2795	319	3.52	0.06	3				-4.2	-4.3	-5.3	0.0%	0.0%	0.0%
ethylene dinitrate	211-063-0	628-96-6	628966	3382	Reach_1462	320	4.31	1.13	3	3.31	1.13		-4.5	-4.3	-5.9	0.0%	0.0%	0.0%
anilinoacetonitrile	221-129-0	3009-97-0	3009970	2585	Reach_1897	321	4.83		1				-3.7	-4.3	-5.8	0.0%	0.0%	0.0%
2-phenoxyethanol	204-589-7	122-99-6	122996	384	Reach_1036	322	5.63	0.25	4	4.44	0.69		-4.5	-4.3	-5.9	0.0%	0.0%	0.0%
disodium [[N,N'-ethylenediylbis[N-(carboxylatomethyl)glycinato]	237-865-0	14025-21-9	14025219	1194	Reach_2355	323	5.52	0.71	4	4.44	0.82		-4.1	-4.3	-5.7	0.0%	0.0%	0.0%
4,4'-methylenedianiline	202-974-4	101-77-9	101779	1328	Reach_582	324	3.99	0.62	3	3.06	0.85		-3.8	-4.3	-6.0	0.0%	0.0%	0.0%
sodium dibutyldithiocarbamate	205-238-0	136-30-1	136301	5676	Reach_1135	325	3.81	1.31	3	2.81	1.31		-4.1	-4.3	-5.7	0.0%	0.0%	0.0%
m-toluidine	601-639-3	119851-28-4	119851284	1700	Reach_4098	326	2.64	0.50	3	1.64	0.50		-4.3	-4.3	-5.9	0.0%	0.0%	0.0%
2,2',2''-(hexahydro-1,3,5-triazine-1,3,5-triyl)triethanol	225-208-0	4719-04-4	4719044	117	Reach_2059	327	4.31	0.53	9	3.48	0.66		-3.4	-4.3	-5.9	0.0%	0.0%	0.0%
potassium sodium tartrate	206-156-8	304-59-6	304596	5833	Reach_1230	328	5.59	0.48	3	4.58	0.66		-4.1	-4.4	-5.7	0.0%	0.0%	0.0%
sodium N-lauroylsarcosinate	205-281-5	137-16-6	137166	5680	Reach_1136	329	4.75	0.26	3	3.70	0.46		-4.1	-4.4	-5.7	0.0%	0.0%	0.0%
17β-hydroxy-17-(3-hydroxypropyl)androst-4-ene-4-one	259-701-7	55542-27-3	55542273	3173	Reach_2808	330	4.50		1				-3.7	-4.4	-5.8	0.0%	0.0%	0.0%
sodium ethylenesulphonate	221-242-5	3039-83-6	3039836	5832	Reach_1903	331	5.44	1.59	3	4.44	1.59		-4.1	-4.4	-5.7	0.0%	0.0%	0.0%
3a,4,7,7a-tetrahydro-4,7-methanoindene	201-052-9	77-73-6	77736	884	Reach_182	332	4.07	0.43	14	3.07	0.43	14	-4.6	-4.4	-5.7	0.0%	0.0%	0.0%
tetrasodium 4,4'-bis[[4-[bis(2-hydroxypropyl)amino]-6-[(4-sulph	267-097-1	67786-25-8	67786258	5986	Reach_2887	333	5.37	0.58	3	4.37	0.58		-4.1	-4.4	-5.7	0.0%	0.0%	0.0%
1-(aminomethyl)cyclohexaneacetic acid hydrochloride	262-075-8	60142-95-2	60142952	5945	Reach_2845	334							-4.1	-4.4	-5.7	0.0%	0.0%	0.0%
N-Pentanoyl-N-{[2'-(1H-tetrazol-5-yl)biphenyl-4-yl]methyl}-L-vali	618-706-8	91161-71-6	91161716	4012	Reach_4498	335	1.78		2				-4.0	-4.4	-5.7	0.0%	0.0%	0.0%
disodium [2,2'-bi-1H-indole]-3,3'-diolate	212-974-6	894-86-0	894860	6077	Reach_1586	336				2.54			-4.1	-4.4	-5.7	0.0%	0.0%	0.0%
aminoiminomethanesulphinic acid	217-157-8	1758-73-2	1758732	2144	Reach_1717	337	5.11	0.42	3	4.26	0.51		-4.1	-4.4	-5.7	0.0%	0.0%	0.0%
2-phenylpropene	202-705-0	98-83-9	98839	4193	Reach_519	338	3.83	0.55	3	3.00	0.72		-4.6	-4.4	-6.0	0.0%	0.0%	0.0%
4-chloro-2-nitroaniline	201-925-4	89-63-4	89634	992	Reach_348	339	3.92	0.70	16	2.92	0.70		-4.2	-4.4	-5.1	0.0%	0.0%	0.0%
benzotriazole	202-394-1	95-14-7	95147	112	Reach_422	340	4.74	0.50	19	3.84	0.63	13	-4.0	-4.4	-5.2	0.0%	0.0%	0.0%
1-butoxypropan-2-ol	225-878-4	5131-66-8	5131668	3032	Reach_2080	341	5.97	0.22	3	4.97	0.22		-4.6	-4.4	-5.6	0.0%	0.0%	0.0%
sodium hydrogen 2-aminobenzene-1,4-disulphonate	214-222-2	1115-20-4	1115204	1550	Reach_1648	342	6.04		2				-4.1	-4.4	-5.7	0.0%	0.0%	0.0%
triphenylphosphine	210-036-0	603-35-0	603350	751	Reach_1412	343	4.31	1.37	3	4.05	0.75		-4.6	-4.4	-5.3	0.0%	0.0%	0.0%
sodium 2,4-dichlorophenoxyacetate	220-290-4	2702-72-9	2702729	1210	Reach_1856	344	5.24	1.00	8	3.99	1.36		-4.1	-4.4	-5.7	0.0%	0.0%	0.0%
2-dimethylaminoethyl methacrylate	220-688-8	2867-47-2	2867472	583	Reach_1878	345	4.66	0.87	4	3.57	1.69		-4.6	-4.4	-5.8	0.0%	0.0%	0.0%
1-ethoxypropan-2-ol	216-374-5	1569-02-4	1569024	2053	Reach_1694	346	6.01	0.64	3	5.01	0.64		-4.6	-4.4	-5.8	0.0%	0.0%	0.0%
3-(methylthio)propionaldehyde	221-882-5	3268-49-3	3268493	2658	Reach_1939	347	3.90	0.42	3	2.90	0.40		-4.6	-4.4	-5.8	0.0%	0.0%	0.0%
n-butyl acetate	204-658-1	123-86-4	123864	397	Reach_1059	348	5.01	0.45	8	4.18	0.78		-4.6	-4.4	-5.9	0.0%	0.0%	0.0%
but-1-ene	203-449-2	106-98-9	106989	1452	Reach_687	349	4.04	0.23	3	3.04	0.23		-4.7	-4.4	-6.8	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
titanium tetrabutanolate	227-006-8	5593-70-4	5593704	5934	Reach_2129	350	6.00	0.33	3	5.00	0.33		-4.1	-4.4	-5.8	0.0%	0.0%	0.0%
4,4'-diaminostilbene-2,2'-disulphonic acid	201-325-2	81-11-8	81118	3801	Reach_271	351	5.10		2				-3.3	-4.4	-6.2	0.0%	0.0%	0.0%
1-methylpiperazine	203-639-5	109-01-3	109013	254	Reach_768	352	6.01	0.32	3	5.01	0.32		-4.6	-4.4	-5.2	0.0%	0.0%	0.0%
2-(2-aminoethylamino)ethanol	203-867-5	111-41-1	111411	1547	Reach_855	353	5.36	0.51	3	4.65	0.57		-3.7	-4.4	-6.1	0.0%	0.0%	0.0%
palmitic acid	200-312-9	57-10-3	57103	3222	Reach_37	354	1.75	0.10	3				-4.5	-4.4	-6.0	0.0%	0.0%	0.0%
hexadecan-1-ol	253-149-0	36653-82-4	36653824	615	Reach_2702	355	5.83		1				-4.5	-4.4	-5.7	0.0%	0.0%	0.0%
1,1'-(ethane-1,2-diyl)bis[pentabromobenzene]	284-366-9	84852-53-9	84852539	3878	Reach_2982	356	4.66	1.81	3	3.66	1.81		-4.6	-4.4	-4.3	0.0%	0.0%	0.0%
succinic acid	203-740-4	110-15-6	110156	274	Reach_805	357	5.09	0.44	3	4.25	0.30		-3.5	-4.4	-6.0	0.0%	0.0%	0.0%
sodium etasulfate	204-812-8	126-92-1	126921	5646	Reach_1091	358	4.98	0.68	3	3.98	0.68		-4.2	-4.4	-5.8	0.0%	0.0%	0.0%
methyl formate	203-481-7	107-31-3	107313	1459	Reach_704	359	6.09	0.76	3	4.68	0.50		-4.7	-4.4	-5.9	0.0%	0.0%	0.0%
menthol	201-939-0	89-78-1	89781	994	Reach_351	360	4.75	0.56	5	3.47	0.28		-4.6	-4.4	-5.8	0.0%	0.0%	0.0%
o-anisidine	201-963-1	90-04-0	90040	999	Reach_357	361	4.33	0.51	4	3.33	0.51		-4.1	-4.4	-6.0	0.0%	0.0%	0.0%
2-(2-aminoethoxy)ethanol	213-195-4	929-06-6	929066	4053	Reach_1603	362	5.43	0.16	3	4.50	0.43		-3.8	-4.4	-6.1	0.0%	0.0%	0.0%
N-cyclohexylbenzothiazole-2-sulfenamide	202-411-2	95-33-0	95330	4125	Reach_426	363	3.81	0.83	3	3.89	1.07		-4.6	-4.4	-6.0	0.0%	0.0%	0.0%
tetrahydrofuran	203-726-8	109-99-9	109999	269	Reach_798	364	6.58	0.30	4	5.58	0.30		-4.7	-4.4	-5.9	0.0%	0.0%	0.0%
(2R,5R)-1,6-Diphenylhexane-2,5-diamine dihydrochloride	203-052-4	102-77-2	102772	1353	Reach_598	365	3.37	0.56	3	2.85	1.07		-4.2	-4.4	-5.8	0.0%	0.0%	0.0%
sodium dimethyldithiocarbamate	204-876-7	128-04-1	128041	1188	Reach_1105	366	3.05	0.94	12	1.23	0.88	3	-4.2	-4.4	-5.8	0.0%	0.0%	0.0%
benzyl(3-hydroxyphenacyl)methylammonium chloride	253-197-2	36768-62-4	36768624	2776	Reach_2704	367	5.16	0.33	3	4.26	0.40		-4.2	-4.4	-5.8	0.0%	0.0%	0.0%
2-chloroethyldiethylammonium chloride	600-382-4	103041-38-9	103041389	1357	Reach_4061	368	4.41	0.92	3				-4.2	-4.4	-5.8	0.0%	0.0%	0.0%
zinc di(benzothiazol-2-yl) disulphide	205-840-3	155-04-4	155044	5716	Reach_1211	369	2.83	0.13	3	1.83	0.13		-4.2	-4.4	-5.8	0.0%	0.0%	0.0%
2-phosphonobutane-1,2,4-tricarboxylic acid	253-733-5	37971-36-1	37971361	2811	Reach_2713	370	6.06	0.89	3	5.06	0.89		-3.4	-4.4	-6.2	0.0%	0.0%	0.0%
N,N'-bis(2,2,6,6-tetramethylpiperidin-4-yl)hexane-1,6-diamine	262-679-1	61260-55-7	61260557	3330	Reach_2849	371	4.90	0.49	3	3.84	0.91		-4.0	-4.4	-5.8	0.0%	0.0%	0.0%
sodium toluene-4-sulphonate	211-522-5	657-84-1	657841	5976	Reach_1490	372	5.50	0.70	3	4.50	0.70		-4.2	-4.4	-5.8	0.0%	0.0%	0.0%
octamethylcyclotetrasiloxane	209-136-7	556-67-2	556672	705	Reach_1368	373	1.90	0.29	6	0.90	0.29		-4.7	-4.4	-6.5	0.0%	0.0%	0.0%
dodecanedioic acid	211-746-3	693-23-2	693232	3538	Reach_1506	374	5.54	1.02	3	4.54	1.02		-4.0	-4.4	-6.1	0.0%	0.0%	0.0%
choline chloride	200-655-4	67-48-1	67481	1231	Reach_81	375	6.09	1.05	3	5.09	1.05		-4.2	-4.4	-5.8	0.0%	0.0%	0.0%
2',4'-dimethylacetoacetanilide	202-576-0	97-36-9	97369	4163	Reach_477	376	5.08		2				-3.8	-4.4	-6.0	0.0%	0.0%	0.0%
decamethylcyclopentasiloxane	208-764-9	541-02-6	541026	3125	Reach_1338	377	2.48	2.14	3	1.48	2.14		-4.6	-4.5	-6.0	0.0%	0.0%	0.0%
2,4-dichloroaniline	607-327-3	24131-07-5	24131075	2375	Reach_4238	378	3.28	0.90	3				-3.8	-4.5	-5.2	0.0%	0.0%	0.0%
sodium 2-methylpropan-2-olate	212-741-9	865-48-5	865485	6066	Reach_1570	379	4.61		1				-4.2	-4.5	-5.8	0.0%	0.0%	0.0%
1-(2-butoxy-1-methylethoxy)propan-2-ol	249-951-5	29911-28-2	29911282	2578	Reach_2637	380	5.68	0.24	3	4.68	0.24		-3.9	-4.5	-6.1	0.0%	0.0%	0.0%
5-chloro-2-(2,4-dichlorophenoxy)aniline	206-017-1	288-13-1	288131	43	Reach_1223	381	6.27	0.68	3	5.27	0.68		-4.0	-4.5	-6.2	0.0%	0.0%	0.0%
5,5-dimethylcyclohexane-1,3-dione	204-804-4	126-81-8	126818	408	Reach_1090	382	7.06		1				-4.1	-4.5	-5.8	0.0%	0.0%	0.0%
1-chloro-2,4-dinitrobenzene	202-551-4	97-00-7	97007	1056	Reach_476	383	2.89	0.65	14	1.89	0.65		-4.7	-4.5	-5.5	0.0%	0.0%	0.0%
oct-1-ene	203-893-7	111-66-0	111660	1553	Reach_864	384	3.32	1.28	3	3.84	2.11		-4.7	-4.5	-6.9	0.0%	0.0%	0.0%
2-methyl-4,6-dinitro-phenol	604-165-5	139893-43-9	139893439	5688	Reach_4143	385							-4.1	-4.5	-5.2	0.0%	0.0%	0.0%
2-[(2-methoxy-4-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxobu	228-768-4	6358-31-2	6358312	3407	Reach_2168	386	2.49	1.73	3				-3.8	-4.5	-5.9	0.0%	0.0%	0.0%
triethyl phosphite	204-552-5	122-52-1	122521	1751	Reach_1030	387	5.93	0.54	3	4.93	0.54		-3.8	-4.5	-6.0	0.0%	0.0%	0.0%
1H-1,2,4-triazole, sodium salt	255-280-9	41253-21-8	41253218	5878	Reach_2741	388	4.88		2				-4.2	-4.5	-5.8	0.0%	0.0%	0.0%
616-083-7	617-435-2	83066-88-0	83066880	950	Reach_4461	389	4.37	0.83	5	4.46	0.84		-4.3	-4.5	-5.5	0.0%	0.0%	0.0%
α,α,α-trifluoro-m-toluidine	202-643-4	98-16-8	98168	1068	Reach_501	390	3.69	0.36	3	2.69	0.36		-4.3	-4.5	-5.4	0.0%	0.0%	0.0%
isoprene	201-143-3	78-79-5	78795	900	Reach_209	391	4.57	0.65	7	3.57	0.65		-4.7	-4.5	-6.7	0.0%	0.0%	0.0%
sebacic acid, compound with hexane-1,6-diamine (1:1)	229-177-4	6422-99-7	6422997	5966	Reach_2183	392							-4.2	-4.5	-5.8	0.0%	0.0%	0.0%
tributyl O-acetylcitrate	201-067-0	77-90-7	77907	3744	Reach_188	393	3.88	0.62	3	2.88	0.62		-4.6	-4.5	-5.9	0.0%	0.0%	0.0%
2,2-dimethylbutyric acid	209-674-2	590-19-2	590192	3264	Reach_1387	394	4.27	0.34	3	3.27	0.34		-4.6	-4.5	-5.2	0.0%	0.0%	0.0%
sodium 3-(allyloxy)-2-hydroxypropanesulphonate	258-004-5	52556-42-0	52556420	5912	Reach_2782	395							-4.2	-4.5	-5.8	0.0%	0.0%	0.0%
[2-(2-methoxymethylethoxy)methylethoxy]propanol	247-045-4	25498-49-1	25498491	2436	Reach_2569	396	6.99	0.25	3	5.99	0.25		-4.5	-4.5	-6.0	0.0%	0.0%	0.0%
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	223-861-6	4098-71-9	4098719	2867	Reach_2013	397	4.26	0.68	3	3.54	0.82		-4.6	-4.5	-5.9	0.0%	0.0%	0.0%
1,1,2-trichloroethane	201-166-9	79-00-5	79005	908	Reach_222	398	4.95	0.70	96	4.23	0.37		-4.8	-4.5	-6.1	0.0%	0.0%	0.0%
Phenol, 4-nonyl-, branched	284-325-5	84852-15-3	84852153	964	Reach_2979	399	2.40	0.84	20	1.67	0.62		-4.6	-4.5	-5.4	0.0%	0.0%	0.0%
1,3-dihydro-5-nitro-2H-benzimidazol-2-one	239-743-2	15667-63-7	15667637	2049	Reach_2392	400	2.38	0.63	3	1.66	0.47		-3.7	-4.5	-6.2	0.0%	0.0%	0.0%
2-propylheptan-1-ol	233-126-1	10042-59-8	10042598	1306	Reach_2278	401	3.41	0.23	3	2.64	0.25		-4.7	-4.5	-5.7	0.0%	0.0%	0.0%
N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine	212-344-0	793-24-8	793248	3771	Reach_1548	402	2.80	1.28	3	2.42	0.42		-4.0	-4.5	-6.1	0.0%	0.0%	0.0%
uronium hydrogen sulphate	244-343-6	21351-39-3	21351393	1205	Reach_2505	403	6.48	0.93	3	4.22	0.39		-4.2	-4.5	-5.8	0.0%	0.0%	0.0%
3,4,5,6-tetrachloro-N-[2-(4,5,6,7-tetrachloro-2,3-dihydro-1,3-dio	250-063-5	30125-47-4	30125474	2587	Reach_2643	404	5.50		3	4.50			-4.3	-4.5	-5.3	0.0%	0.0%	0.0%
docosan-1-ol	211-546-6	661-19-8	661198	3464	Reach_1491	405	-0.15	0.62	3				-4.4	-4.5	-5.0	0.0%	0.0%	0.0%
2-diethylaminoethanol	202-845-2	100-37-8	100378	123	Reach_553	406	5.46	0.70	4	4.17	0.54		-4.7	-4.5	-5.7	0.0%	0.0%	0.0%
4-nitroaniline	201-208-6	79-44-7	79447	3777	Reach_246	407	4.43	1.60	3				-4.1	-4.5	-5.3	0.0%	0.0%	0.0%
617-435-2	616-083-7	74351-78-3	74351783	3634	Reach_4422	408	2.85	1.02	3				-4.4	-4.5	-5.3	0.0%	0.0%	0.0%
dimethyl carbonate	210-478-4	616-38-6	616386	3345	Reach_1431	409	5.46	0.30	3	4.46	0.30		-4.7	-4.5	-5.7	0.0%	0.0%	0.0%
neodecanoic acid	248-093-9	26896-20-8	26896208	2491	Reach_2595	410	5.09	0.35	3	4.09	0.35		-4.7	-4.5	-6.1	0.0%	0.0%	0.0%
12-hydroxystearic acid	203-366-1	106-14-9	106149	1429	Reach_656	411	2.09	0.19	3				-3.9	-4.5	-6.0	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
diuron (reach)	206-354-4	330-54-1	330541	46	Reach_1238	412	2.82	1.26	86	1.27	1.02	23	-4.1	-4.5	-5.3	0.0%	0.0%	0.0%
salicylic acid	200-712-3	69-72-7	69727	84	Reach_95	413	5.24	1.02	7	4.15	0.57		-4.0	-4.5	-6.1	0.0%	0.0%	0.0%
N-butylbenzenesulphonamide	222-823-6	3622-84-2	3622842	2763	Reach_1977	414	4.71	0.13	3	3.71	0.13		-4.5	-4.5	-6.0	0.0%	0.0%	0.0%
N-carboxymethyliminobis(ethylenenitrilo)tetra(acetic acid)	200-652-8	67-43-6	67436	82	Reach_80	415	5.19	0.99	4	4.64	1.00		-3.7	-4.5	-5.7	0.0%	0.0%	0.0%
4-aminophenol	204-616-2	123-30-8	123308	386	Reach_1044	416	2.42	0.84	20	1.84	0.84		-3.8	-4.5	-6.0	0.0%	0.0%	0.0%
calcium 4-[(5-chloro-4-methyl-2-sulphonatophenyl)azo]-3-hydro	230-303-5	7023-61-2	7023612	6004	Reach_2220	417	5.05	0.91	3	4.05	0.91		-4.2	-4.5	-5.9	0.0%	0.0%	0.0%
612-012-9	205-334-2	138-59-0	138590	445	Reach_1141	418	4.93	0.75	6	3.93	0.75		-4.4	-4.5	-5.5	0.0%	0.0%	0.0%
4-[(2,5-dichlorophenyl)azo]-3-hydroxy-2-naphthoic acid	237-913-0	14064-10-9	14064109	450	Reach_2356	419	3.88	0.86	3	2.88	0.86		-4.4	-4.5	-5.6	0.0%	0.0%	0.0%
2-ethylhexyl acrylate	203-080-7	103-11-7	103117	159	Reach_602	420	4.13	0.58	5	2.87	0.49		-4.7	-4.5	-6.0	0.0%	0.0%	0.0%
ethylene carbonate	202-510-0	96-49-1	96491	4149	Reach_467	421	7.27	0.42	3	6.27	0.42		-4.3	-4.5	-6.2	0.0%	0.0%	0.0%
tetramethylsilane	200-899-1	75-76-3	75763	3685	Reach_160	422	3.07	1.46	3	2.07	1.46		-5.0	-4.5	-6.8	0.0%	0.0%	0.0%
sodium methanethiolate	225-969-9	5188-07-8	5188078	5582	Reach_2084	423	3.58	0.39	3	2.58	0.39		-4.3	-4.5	-5.9	0.0%	0.0%	0.0%
(R)-lactic acid	245-247-7	22818-40-2	22818402	2339	Reach_2524	424	4.17	0.72	3				-3.7	-4.5	-6.1	0.0%	0.0%	0.0%
2-chlorobenzaldehyde	201-956-3	89-98-5	89985	997	Reach_355	425	3.87	0.35	6	2.87	0.35		-4.7	-4.5	-5.5	0.0%	0.0%	0.0%
isooctene	234-294-9	11071-47-9	11071479	1529	Reach_2303	426	3.88	0.32	3	2.88	0.32		-4.8	-4.5	-7.0	0.0%	0.0%	0.0%
dodecamethylcyclohexasiloxane	208-762-8	540-97-6	540976	3124	Reach_1337	427	1.45	0.59	3	0.45	0.59		-4.7	-4.5	-5.5	0.0%	0.0%	0.0%
[ethylenebis[nitrilobis(methylene)]]tetrakisphosphonic acid, calc	287-370-9	85480-89-3	85480893	6060	Reach_2985	428	5.58	0.42	3	4.58	0.42		-4.3	-4.5	-5.9	0.0%	0.0%	0.0%
ethyl acrylate	205-438-8	140-88-5	140885	452	Reach_1151	429	3.64	0.43	5	2.89	0.50		-4.8	-4.5	-5.9	0.0%	0.0%	0.0%
chlorodifluoromethane	200-871-9	75-45-6	75456	3673	Reach_145	430	5.67	0.18	3	4.67	0.18		-5.1	-4.5	-6.8	0.0%	0.0%	0.0%
phenazone	200-486-6	60-80-0	60800	74	Reach_59	431							-4.2	-4.5	-5.3	0.0%	0.0%	0.0%
disodium phthalate	240-106-6	15968-01-1	15968011	5728	Reach_2406	432	5.35	0.60	3	4.63	0.46		-4.3	-4.5	-5.9	0.0%	0.0%	0.0%
2-pyridylamine	207-988-4	504-29-0	504290	658	Reach_1304	433	4.29	0.76	5	3.29	0.75		-4.7	-4.5	-5.3	0.0%	0.0%	0.0%
603-434-4	203-729-4	110-02-1	110021	272	Reach_801	434	4.78	0.53	4	3.78	0.53		-4.4	-4.5	-5.6	0.0%	0.0%	0.0%
cyclohexyl phenyl ketone	211-923-5	712-50-5	712505	818	Reach_1520	435	3.71	0.23	3	2.71	0.23		-4.8	-4.5	-5.6	0.0%	0.0%	0.0%
tetrasodium 4,4'-{ethene-1,2-diylbis[(3-sulfonato-4,1-phenylene	218-414-7	2146-71-6	2146716	2295	Reach_1764	436	4.73	1.51	3	3.73	1.51		-4.3	-4.5	-5.9	0.0%	0.0%	0.0%
hexane-1,6-diol	211-074-0	629-11-8	629118	3385	Reach_1464	437	6.54	0.32	3	5.54	0.32		-3.9	-4.5	-6.1	0.0%	0.0%	0.0%
2,3-xylidine	617-346-9	82543-15-5	82543155	3828	Reach_4454	438	4.69		1				-4.7	-4.5	-5.3	0.0%	0.0%	0.0%
biphenyl-4-ol	202-179-2	92-69-3	92693	1013	Reach_388	439	3.48	0.34	3	2.48	0.34		-4.5	-4.5	-5.6	0.0%	0.0%	0.0%
N-ethylaniline	203-135-5	103-69-5	103695	162	Reach_611	440	4.39	0.65	7	3.39	0.65		-4.8	-4.5	-5.3	0.0%	0.0%	0.0%
cycloheptapentylose	231-493-2	7585-39-9	7585399	6405	Reach_2263	441	5.89	0.83	3	4.89	0.83		-4.3	-4.5	-5.9	0.0%	0.0%	0.0%
lactonitrile	201-163-2	78-97-7	78977	3762	Reach_220	442	2.80	0.92	3	1.77	0.46		-4.2	-4.5	-6.2	0.0%	0.0%	0.0%
Disodium 4-amino-3-[{4-[({4-[(2,4-diaminophenyl)diazenyl]phen	605-104-5	157577-99-6	157577996	5722	Reach_4167	443	5.45	1.40	3	4.45	1.40		-4.3	-4.5	-5.9	0.0%	0.0%	0.0%
allyl alcohol	203-470-7	107-18-6	107186	213	Reach_697	444	3.28	0.66	19	2.59	0.80	12	-4.7	-4.5	-6.0	0.0%	0.0%	0.0%
2-methoxy-1-methylethyl acetate	203-603-9	108-65-6	108656	1487	Reach_750	445	5.94	0.49	3	4.94	0.49		-4.7	-4.6	-6.0	0.0%	0.0%	0.0%
3-aminopropyldimethylamine	203-680-9	109-55-7	109557	1503	Reach_777	446	5.06	0.91	3	4.17	0.94		-4.7	-4.6	-6.1	0.0%	0.0%	0.0%
thymol	224-832-0	4511-42-6	4511426	2938	Reach_2045	447	5.75	0.50	3	5.14	0.48		-4.8	-4.6	-5.5	0.0%	0.0%	0.0%
disodium 2,2'-([1,1'-biphenyl]-4,4'-diyldivinylene)bis(benzenesul	248-421-0	27344-41-8	27344418	1212	Reach_2602	448	4.84	0.44	4	4.22	0.74		-4.3	-4.6	-5.9	0.0%	0.0%	0.0%
sodium O-ethyl dithiocarbonate	205-440-9	140-90-9	140909	1196	Reach_1153	449	3.73	1.06	5	4.37	1.01		-4.3	-4.6	-5.9	0.0%	0.0%	0.0%
propazine (reach)	205-359-9	139-40-2	139402	446	Reach_1144	450	4.00	1.05	10	1.82	0.87		-4.4	-4.6	-5.3	0.0%	0.0%	0.0%
trisodium 2-(carboxylatomethyl(2-hydroxyethyl)amino)ethylimir	205-381-9	139-89-9	139899	5689	Reach_1145	451	5.05	1.05	3	4.52	1.18		-4.3	-4.6	-5.9	0.0%	0.0%	0.0%
L-Cysteine, hydrochloride, hydrate	615-117-8	7048-04-6	7048046	5585	Reach_4410	452							-4.3	-4.6	-5.9	0.0%	0.0%	0.0%
sodium sulphanilate	208-208-5	515-74-2	515742	5906	Reach_1319	453							-4.3	-4.6	-5.9	0.0%	0.0%	0.0%
triacetin	203-051-9	102-76-1	102761	1352	Reach_597	454	5.66	0.45	3	4.66	0.45		-4.5	-4.6	-6.2	0.0%	0.0%	0.0%
potassium (R)-[(3-ethoxy-1-methyl-3-oxoprop-1-enyl)amino]phe	213-510-5	961-69-3	961693	6093	Reach_1620	455							-4.3	-4.6	-5.9	0.0%	0.0%	0.0%
2-(2-butoxyethoxy)ethyl acetate	204-685-9	124-17-4	124174	1787	Reach_1071	456	5.54	0.57	3	4.54	0.57		-4.8	-4.6	-6.1	0.0%	0.0%	0.0%
ethylamine	200-834-7	75-04-7	75047	846	Reach_125	457	5.26	0.67	4	3.98	0.60		-4.8	-4.6	-5.6	0.0%	0.0%	0.0%
2-(2-(2-butoxyethoxy)ethoxy)ethanol	205-592-6	143-22-6	143226	1959	Reach_1190	458	6.24	0.32	4	5.54	0.51		-3.8	-4.6	-6.3	0.0%	0.0%	0.0%
4-methyloxazole-5-carbonitrile	214-029-3	1073-69-4	1073694	1461	Reach_1643	459	3.03	0.74	3	2.03	0.74		-3.7	-4.6	-6.2	0.0%	0.0%	0.0%
octadec-1-ene	204-012-9	112-88-9	112889	1609	Reach_928	460	3.32	1.28	3	3.84	2.09		-4.5	-4.6	-5.8	0.0%	0.0%	0.0%
2-(dimethylamino)ethyl acrylate	219-460-0	2439-35-2	2439352	2391	Reach_1811	461	3.58	0.87	3	2.65	1.21		-4.8	-4.6	-6.0	0.0%	0.0%	0.0%
4,4'-methylenebis[2-chloroaniline]	202-918-9	101-14-4	101144	1315	Reach_573	462	3.20	0.26	3	2.20	0.26		-4.1	-4.6	-6.2	0.0%	0.0%	0.0%
γ-butyrolactone	202-509-5	96-48-0	96480	4148	Reach_466	463	5.59	0.62	3	4.59	0.62		-4.7	-4.6	-6.2	0.0%	0.0%	0.0%
disodium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4-)-N,	237-864-5	14025-15-1	14025151	1193	Reach_2354	464	5.58	0.71	4	4.43	0.84		-4.3	-4.6	-5.9	0.0%	0.0%	0.0%
tetrachloroethylene	204-825-9	127-18-4	127184	20	Reach_1096	465	4.28	0.66	16	3.87	0.92	7	-4.8	-4.6	-6.6	0.0%	0.0%	0.0%
sodium dihydrogen citrate	242-734-6	18996-35-5	18996355	5752	Reach_2473	466	6.34	0.41	3	5.34	0.41		-4.3	-4.6	-5.9	0.0%	0.0%	0.0%
2,2',6,6'-Tetrabromo-4,4'-isopropylidenediphenol, oligomeric rea	500-107-7	40039-93-8	40039938	5873	Reach_4053	467				1.36			-4.3	-4.6	-5.9	0.0%	0.0%	0.0%
sodium 2-ethylhexanoate	243-283-8	19766-89-3	19766893	5763	Reach_2484	468	5.28	0.45	3	4.42	0.29		-4.3	-4.6	-5.9	0.0%	0.0%	0.0%
2-methoxyethanol	203-713-7	109-86-4	109864	267	Reach_794	469	6.85	0.71	9	5.27	0.70		-4.8	-4.6	-6.2	0.0%	0.0%	0.0%
zirconium acetate	231-492-7	7585-20-8	7585208	6028	Reach_2262	470	4.77		1				-4.3	-4.6	-5.9	0.0%	0.0%	0.0%
hexasodium 2,2'-[vinylenebis[(3-sulphonato-4,1-phenylene)imin	273-468-9	68971-49-3	68971493	6000	Reach_2914	471				4.16			-4.3	-4.6	-6.0	0.0%	0.0%	0.0%
zinc bis(dibenzyldithiocarbamate)	238-778-0	14726-36-4	14726364	5701	Reach_2368	472	2.68	0.71	3	1.68	0.71		-4.3	-4.6	-6.0	0.0%	0.0%	0.0%
carbon disulphide	200-843-6	75-15-0	75150	852	Reach_132	473	4.00	0.71	7	3.00	0.63		-4.8	-4.6	-6.6	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
pentaerithrityl tetranitrate	201-084-3	78-11-5	78115	892	Reach_194	474	5.37	0.64	3	4.37	0.64		-4.0	-4.6	-6.0	0.0%	0.0%	0.0%
diammonium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4	270-232-7	68413-60-5	68413605	5997	Reach_2906	475	5.27	0.24	3	4.27	0.24		-4.3	-4.6	-6.0	0.0%	0.0%	0.0%
ethylenediaminetetraacetonitrile	227-290-3	5766-67-6	5766676	3236	Reach_2135	476	5.33	0.38	3	4.33	0.38		-3.7	-4.6	-6.2	0.0%	0.0%	0.0%
sodium O-isobutyl dithiocarbonate	246-805-2	25306-75-6	25306756	1209	Reach_2564	477	4.40	0.77	5	4.00	0.63		-4.3	-4.6	-5.9	0.0%	0.0%	0.0%
chlorotrimethylsilane	200-900-5	75-77-4	75774	3686	Reach_161	478	5.50	0.25	3	4.46	0.30		-5.1	-4.6	-6.8	0.0%	0.0%	0.0%
toluenesulphonamide	215-578-1	1333-07-9	1333079	1866	Reach_1678	479	5.22	0.28	3	4.38	0.87		-4.1	-4.6	-6.2	0.0%	0.0%	0.0%
sodium prop-2-enesulphonate	219-676-5	2495-39-8	2495398	5793	Reach_1823	480	6.66		1				-4.4	-4.6	-5.9	0.0%	0.0%	0.0%
5H-dibenz[b,f]azepine	209-798-7	593-56-6	593566	1226	Reach_1394	481	2.80	0.25	4	2.30	0.26		-4.3	-4.6	-6.1	0.0%	0.0%	0.0%
1,2,4-triazole	206-022-9	288-88-0	288880	584	Reach_1224	482	5.39	0.70	5	4.65	1.03		-3.7	-4.6	-6.3	0.0%	0.0%	0.0%
[nitrilotris(methylene)]trisphosphonic acid, sodium salt	243-900-0	20592-85-2	20592852	2271	Reach_2496	483	5.62	0.42	3	4.62	0.42		-3.7	-4.6	-6.2	0.0%	0.0%	0.0%
butene	246-689-3	25167-67-3	25167673	2419	Reach_2560	484	4.05	0.20	3	3.05	0.20		-4.9	-4.6	-7.0	0.0%	0.0%	0.0%
2-amino-4,5-dichlorobenzenesulfonic acid	700-372-0	1128026-41-4	1128026414	1604	Reach_4877	485	4.54		1				-3.8	-4.6	-5.9	0.0%	0.0%	0.0%
m-xylene	203-576-3	108-38-3	108383	236	Reach_742	486	3.99	0.48	17	2.99	0.70	68	-4.9	-4.6	-6.6	0.0%	0.0%	0.0%
4-chlorobenzonitrile	244-870-1	22252-43-3	22252433	2326	Reach_2520	487	5.09	1.11	3				-4.8	-4.6	-5.5	0.0%	0.0%	0.0%
diguanidinium carbonate	209-813-7	593-85-1	593851	5942	Reach_1397	488	5.02	0.81	3	4.02	0.81		-4.4	-4.6	-6.0	0.0%	0.0%	0.0%
6-hydroxy-1H-pyrimidin-4-one	214-772-3	1193-24-4	1193244	1690	Reach_1671	489	4.65		2				-3.9	-4.6	-6.1	0.0%	0.0%	0.0%
4-amino-2,5-dichlorobenzenesulphonic acid	263-560-7	62476-59-9	62476599	1228	Reach_2853	490	4.80	0.62	11	3.80	0.62	11	-3.8	-4.6	-5.9	0.0%	0.0%	0.0%
nicotinamide	202-713-4	98-92-0	98920	1079	Reach_524	491	6.50	0.31	3	5.50	0.31		-3.8	-4.6	-6.1	0.0%	0.0%	0.0%
potassium mercaptoacetate	252-038-4	34452-51-2	34452512	5852	Reach_2679	492	5.07	0.89	3	4.07	0.89		-4.4	-4.6	-6.0	0.0%	0.0%	0.0%
2-ethylhexyl nitrate	248-363-6	27247-96-7	27247967	2497	Reach_2599	493	3.39		2				-4.8	-4.6	-6.0	0.0%	0.0%	0.0%
ammonium mercaptoacetate	226-540-9	5421-46-5	5421465	5923	Reach_2109	494	5.07	0.89	3	4.07	0.89		-4.4	-4.6	-6.0	0.0%	0.0%	0.0%
(methoxymethyl)triphenylphosphonium chloride	204-077-3	115-27-5	115275	1635	Reach_941	495	5.29	0.28	3	4.29	0.28		-4.4	-4.6	-6.0	0.0%	0.0%	0.0%
2-isopropoxyethanol	203-685-6	109-59-1	109591	257	Reach_778	496	6.31	0.52	4	5.31	0.52		-4.8	-4.6	-5.5	0.0%	0.0%	0.0%
2,2,6,6-tetramethyl-4-piperidone	212-554-2	826-36-8	826368	3834	Reach_1556	497	5.28	0.52	3	4.14	0.69		-4.8	-4.6	-5.9	0.0%	0.0%	0.0%
biphenyl-4,4'-diol	202-200-5	92-88-6	92886	1015	Reach_395	498	3.61	0.44	3	2.61	0.44		-4.0	-4.6	-5.8	0.0%	0.0%	0.0%
1,2-dichloropropane	201-152-2	78-87-5	78875	902	Reach_213	499	5.00	0.48	10	4.24	0.55		-4.9	-4.6	-6.4	0.0%	0.0%	0.0%
barium bis[2-chloro-5-[(2-hydroxy-1-naphthyl)azo]toluene-4-sul	225-935-3	5160-02-1	5160021	5581	Reach_2081	500	4.97	1.01	3	3.97	1.01		-4.4	-4.6	-6.0	0.0%	0.0%	0.0%
2-butene	203-452-9	107-01-7	107017	1454	Reach_689	501	4.17	0.27	3	3.17	0.27		-4.9	-4.6	-7.3	0.0%	0.0%	0.0%
ametryn (reach)	212-634-7	834-12-8	834128	953	Reach_1562	502	3.09	1.19	35	1.56	1.27	7	-4.4	-4.6	-5.4	0.0%	0.0%	0.0%
methyltriphenylphosphonium bromide	201-056-0	77-76-9	77769	3735	Reach_184	503	5.06	0.71	3				-4.4	-4.6	-6.0	0.0%	0.0%	0.0%
cyclohex-1,2-ylenediamine	211-776-7	694-83-7	694837	807	Reach_1510	504	5.00	0.77	3	4.00	0.77		-4.7	-4.6	-5.7	0.0%	0.0%	0.0%
2-methylpropan-1-ol	201-148-0	78-83-1	78831	901	Reach_210	505	6.04	0.70	76	5.04	0.70		-4.8	-4.6	-6.0	0.0%	0.0%	0.0%
benzene-1,2,4-tricarboxylic acid 1,2-anhydride	209-008-0	552-30-7	552307	3164	Reach_1358	506	5.50	0.31	3				-4.0	-4.6	-6.2	0.0%	0.0%	0.0%
[ethylenebis[nitrilobis(methylene)]]tetrakisphosphonic acid, sod	244-742-5	22036-77-7	22036777	5776	Reach_2513	507	6.11		2	4.80			-4.4	-4.6	-6.0	0.0%	0.0%	0.0%
Amines, bis(hydrogenated tallow alkyl), 2-[[bis(hydrogenated tal	294-705-2	91745-35-6	91745356	6407	Reach_2995	508	5.50		3	4.50			-4.4	-4.6	-6.0	0.0%	0.0%	0.0%
sodium decyl sulphate	205-568-5	142-87-0	142870	5696	Reach_1182	509	4.87	1.23	3	3.86	1.40		-4.4	-4.6	-6.0	0.0%	0.0%	0.0%
ammonium myristate	240-599-8	16530-71-5	16530715	5734	Reach_2424	510							-4.4	-4.6	-6.0	0.0%	0.0%	0.0%
dioctadecyl 3,3'-thiodipropionate	211-750-5	693-36-7	693367	3539	Reach_1507	511	5.19	0.73	3	4.19	0.73		-4.8	-4.6	-3.1	0.0%	0.0%	0.1%
Castor oil, hydrogenated, lithium salt	265-222-4	64754-95-6	64754956	6402	Reach_2866	512	5.52		3	4.52			-4.4	-4.6	-6.0	0.0%	0.0%	0.0%
methyl acrylate	202-500-6	96-33-3	96333	1053	Reach_462	513	3.74	0.40	5	2.82	0.44		-4.9	-4.6	-6.0	0.0%	0.0%	0.0%
potassium sulphanilate	213-834-7	1025-15-6	1025156	1343	Reach_1635	514	5.53		1				-4.4	-4.6	-6.0	0.0%	0.0%	0.0%
4,5,6,7-tetrahydrothieno[3,2-c]pyridinium chloride	246-073-4	24199-46-0	24199460	2376	Reach_2540	515	4.62	0.32	3	3.62	0.32		-4.4	-4.6	-6.0	0.0%	0.0%	0.0%
disodium [N,N-bis[2-[bis(carboxymethyl)amino]ethyl]glycinato(5	243-136-8	19529-38-5	19529385	5762	Reach_2481	516	5.34	1.09	3	5.19	0.33		-4.4	-4.6	-6.0	0.0%	0.0%	0.0%
butanone oxime	202-496-6	96-29-7	96297	1051	Reach_459	517	5.39	0.87	4	4.35	1.08		-4.9	-4.6	-5.8	0.0%	0.0%	0.0%
piperazine	203-808-3	110-85-0	110850	1531	Reach_832	518	4.32		1	4.40			-4.7	-4.7	-6.4	0.0%	0.0%	0.0%
N-butyl-2,2,6,6-tetramethylpiperidin-4-amine	252-899-6	36177-92-1	36177921	2761	Reach_2698	519	4.48	0.74	3	3.48	0.74		-4.8	-4.7	-6.1	0.0%	0.0%	0.0%
docosyltrimethylammonium methyl sulphate	279-791-1	81646-13-1	81646131	6043	Reach_2960	520	3.21	0.56	3	2.21	0.56		-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
2,2'-methyliminodiethanol	203-312-7	105-59-9	105599	1416	Reach_645	521	5.47	0.59	3	4.49	0.78		-3.9	-4.7	-6.3	0.0%	0.0%	0.0%
trisodium bis[3-hydroxy-4-[(2-hydroxy-1-naphthyl)azo]-7-nitrona	260-906-9	57693-14-8	57693148	5938	Reach_2826	522	4.37	0.51	3	3.37	0.51		-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
stearic acid	200-313-4	57-11-4	57114	3223	Reach_38	523	1.31	0.36	3				-4.7	-4.7	-6.2	0.0%	0.0%	0.0%
2,2'-dimethyl-2,2'-azodipropiononitrile	201-132-3	78-67-1	78671	3754	Reach_203	524	4.42	0.55	3	3.42	0.55		-4.9	-4.7	-6.1	0.0%	0.0%	0.0%
glyoxylic acid	206-058-5	298-12-4	298124	2573	Reach_1228	525	5.30	0.50	3	4.30	0.50		-3.7	-4.7	-6.3	0.0%	0.0%	0.0%
2,3-dichloropyridine	200-624-5	66-25-1	66251	788	Reach_78	526	4.24	0.75	4	3.24	0.75		-4.1	-4.7	-6.0	0.0%	0.0%	0.0%
4-chloro-2,5-dimethoxyaniline	228-782-0	6358-64-1	6358641	3409	Reach_2170	527	4.20	0.74	3	3.20	0.74		-4.1	-4.7	-6.2	0.0%	0.0%	0.0%
sodium 1,4-bis(1,3-dimethylbutyl) sulphonatosuccinate	219-147-9	2373-38-8	2373388	5788	Reach_1789	528	6.06		1				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
lauric acid	205-582-1	143-07-7	143077	468	Reach_1188	529	4.37	0.57	7	3.37	0.57		-4.7	-4.7	-6.3	0.0%	0.0%	0.0%
cysteine hydrochloride	200-157-7	52-89-1	52891	5917	Reach_17	530	5.22	0.50	3	4.22	0.50		-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
sodium 3-nitrobenzenesulphonate	204-857-3	127-68-4	127684	5650	Reach_1101	531	6.64	0.35	3	5.64	0.35		-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
allyl 2,3-epoxypropyl ether	203-442-4	106-92-3	106923	201	Reach_682	532	4.89	0.48	4	3.79	0.38		-4.9	-4.7	-5.7	0.0%	0.0%	0.0%
6-ethyl-2-toluidine	247-323-5	25899-50-7	25899507	2446	Reach_2571	533	5.08	0.37	3	4.08	0.37		-4.2	-4.7	-6.3	0.0%	0.0%	0.0%
benzenesulphonic acid	202-638-7	98-11-3	98113	4179	Reach_499	534	5.62		2				-3.8	-4.7	-6.2	0.0%	0.0%	0.0%
1,3-dichloro-4-nitrobenzene	203-687-7	109-61-5	109615	1504	Reach_780	535	4.14	1.69	3	3.14	1.69		-4.9	-4.7	-5.7	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
isobutyraldehyde	201-149-6	78-84-2	78842	3759	Reach_211	536	4.95	0.45	3	3.95	0.45		-4.9	-4.7	-6.1	0.0%	0.0%	0.0%
Ethyl (2S)-2-({[(2-isopropyl-1,3-thiazol-4-yl)methyl](methyl)carba	931-074-0	1247119-36-3	1247119363	5641	Reach_5130	537							-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
2-ethylhexyl oleate	247-655-0	26399-02-0	26399020	2468	Reach_2581	538	6.35	1.10	3	5.35	1.10		-4.8	-4.7	-5.2	0.0%	0.0%	0.0%
propargite	219-006-1	2312-35-8	2312358	548	Reach_1783	539	3.64	1.44	19	1.35	1.05	8	-4.3	-4.7	-5.5	0.0%	0.0%	0.0%
sodium 4-(4-methyl-3-nitrobenzoylamino)benzenesulphonate	281-719-9	84029-45-8	84029458	6049	Reach_2969	540							-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
bis(2-ethylhexyl) terephthalate	229-176-9	6422-86-2	6422862	3430	Reach_2182	541	3.87	2.07	3	2.87	2.07		-4.6	-4.7	-5.8	0.0%	0.0%	0.0%
[[(phosphonomethyl)imino]bis[ethylenenitrilobis(methylene)]]te	274-798-6	70714-66-8	70714668	6006	Reach_2920	542	6.07		2	4.70			-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
sodium (5s,8s)-8-methoxy-2,4-dioxo-1,3-diazaspiro[4.5]decan-3-	929-513-6	1400584-86-2	1400584862	5690	Reach_5126	543							-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
691-746-1	937-694-8	15295-77-9	15295779	5713	Reach_5145	544							-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
614-977-1	204-973-4	130-00-7	130007	1831	Reach_1115	545	3.63		1				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
2-(chloromethyl)-3-methyl-4-(2,2,2-trifluoroethoxy)pyridine hyd	700-531-4	1093205-93-6	1093205936	1498	Reach_4925	546	3.42	1.80	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
N-[2-(3-carbamoyl-4-hydroxyphenyl)-2-oxoethyl]-N-(4-phenylbu	700-288-4	96441-14-4	96441144	6094	Reach_4843	547							-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
6,6'-[(3,3'-di-tert-butyl-5,5'-dimethoxybiphenyl-2,2'-diyl)bis(oxy)	204-979-7	130-17-6	130176	1833	Reach_1117	548	4.13	0.24	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
607-657-8	687-783-8	13222-26-9	13222269	1855	Reach_4637	549	4.68	0.52	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
3-chloropropyldimethylammonium chloride	700-022-7	13349-82-1	13349821	1867	Reach_4127	550	5.07	1.00	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
[2-(4-benzyl-2-phenylpiperazin-1-yl)phenyl]methanol (2E)-but-2-	205-066-6	132-57-0	132570	1860	Reach_1123	551	4.86	0.31	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
604-165-5	617-251-2	816431-72-8	816431728	3809	Reach_4448	552	5.40		1				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
(3aR,8aS,8bS)-1,3-Dibenzyl-2-oxodecahydrothieno[1',2':1,2]thier	286-111-7	85187-23-1	85187231	3884	Reach_2983	553	2.35	0.49	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
(2-ethoxy-1-methyl-2-oxoethyl)triphenylphosphonium bromide	211-838-3	700-13-0	700130	3554	Reach_1515	554	3.43	0.53	3	2.66	0.54		-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
methyl (2S-trans)-6,8-dideoxy-6-[[(1-methyl-4-propylpyrrolidin-2	201-475-9	83-42-1	83421	954	Reach_282	555	3.87	0.70	24	3.08	0.70		-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
disodium 4,4'-methylenebis[3-hydroxy-2-naphthoate]	620-109-2	77820-58-7	77820587	3737	Reach_4558	556	4.41	0.43	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
2-chloroethyldimethylammonium chloride	256-350-1	48076-38-6	48076386	2970	Reach_2759	557	0.64	1.80	3	5.00			-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
611-624-3	241-293-7	17261-28-8	17261288	2129	Reach_2431	558	4.68		2				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
(2,4-diaminopteridin-6-yl)methanol monohydrochloride	700-274-8	73978-41-3	73978413	6019	Reach_4834	559							-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
(2S)-N-[(diethylamino)methyl]-2-(2-oxopyrrolidin-1-yl)butanamic	692-514-2	133047-57-1	133047571	1865	Reach_4676	560							-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
(3S)-N,N-dimethyl-3-(naphthalen-1-yloxy)-3-(thiophen-2-yl)prop	236-412-4	13360-57-1	13360571	1868	Reach_2329	561	5.84	0.79	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
Salt of N-acetyl-L-glutamic acid and 1-[(7S)-3,4-dimethoxybicyclc	603-772-2	133865-89-1	133865891	1871	Reach_4129	562	4.00	0.61	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
N-methylhyoscinium bromide	206-340-8	328-99-4	328994	2667	Reach_1236	563	3.57	1.11	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
hyoscine hydrobromide	619-590-1	135302-13-5	135302135	1888	Reach_4531	564	5.50		3	4.50			-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
sodium 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoate	201-920-7	89-58-7	89587	3981	Reach_346	565	4.17	0.45	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
692-713-4	619-328-6	98231-71-1	98231711	6095	Reach_4514	566							-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
2-[tert-butyl(phenylmethyl)amino]-1-[4-hydroxy-3-(hydroxymetl	619-779-9	120100-77-8	120100778	1704	Reach_4544	567	5.53	0.30	3	4.53	0.30		-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
5-aminopyrazole-4-carboxamide hemisulphate	208-610-0	535-13-7	535137	3105	Reach_1333	568	4.67	1.72	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
1-{[2-(2,4-difluorophenyl)oxiran-2-yl]methyl}-1H-1,2,4-triazole m	603-957-8	13636-02-7	13636027	1898	Reach_4134	569	4.21	0.78	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
616-640-4	692-713-4	886588-62-1	886588621	6075	Reach_4678	570							-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
(2-carbamimidamido-1,3-thiazol-4-yl)methyl carbamimidothioat	205-289-9	137-32-6	137326	1907	Reach_1138	571	5.50	0.33	3	4.50	0.33		-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
600-588-4	237-307-6	13734-41-3	13734413	1908	Reach_2347	572	4.44	0.97	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
4,4,13,13-tetraethoxy-3,14-dioxa-8,9-dithia-4,13-disilahexadecar	260-350-7	56706-10-6	56706106	3209	Reach_2819	573	5.42	1.31	3	4.42	1.31		-4.8	-4.7	-6.2	0.0%	0.0%	0.0%
611-000-0	220-635-9	2840-28-0	2840280	2529	Reach_1874	574	3.99	0.68	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
benzyldimethyl[2-[(1-oxoallyl)oxy]ethyl]ammonium chloride	609-118-2	353497-37-7	353497377	2730	Reach_4290	575	3.54	0.83	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
619-328-6	700-178-6	121627-17-6	121627176	6393	Reach_4793	576	4.38		1				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
8-benzyl-3-oxo-8-azoniabicyclo[3.2.1]octane chloride	696-512-2	1378387-81-5	1378387815	1912	Reach_4718	577	4.78	1.77	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
1-(2-isopropyl-1,3-thiazol-4-yl)-N-methylmethanamine dihydroc	604-047-3	137863-20-8	137863208	1913	Reach_4139	578	4.70	0.39	3	3.70	0.39		-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
N,N,N-trimethyladamantan-1-aminium chloride	250-550-2	31291-60-8	31291608	2623	Reach_2653	579	2.64	0.32	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
603-758-6	610-029-6	4245-76-5	4245765	2892	Reach_4320	580	5.40	0.15	3	4.40	0.15		-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
617-892-8	212-090-0	761-65-9	761659	871	Reach_1533	581	4.95		2				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
N-(aminosulfonyl)-3-chloropropanimidamide hydrochloride	604-112-6	139147-73-2	139147732	1917	Reach_4142	582	4.08		2				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
glucosamine hydrochloride	642-256-1	139481-58-6	139481586	1920	Reach_4610	583	3.11	0.96	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
Potassium 4-methylbenzenesulfinate	205-410-5	140-29-4	140294	1926	Reach_1148	584	5.04	0.63	3	4.04	0.63		-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
lysine hydrochloride	230-356-4	7065-46-5	7065465	2117	Reach_2221	585	4.47	0.48	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
(3S)-2-Oxotetrahydrofuran-3-ammonium bromide	604-254-9	141818-73-7	141818737	1943	Reach_4145	586	4.05	0.60	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
cefazolin	601-332-4	114882-16-5	114882165	1627	Reach_4085	587	3.11	0.15	3				-3.8	-4.7	-6.0	0.0%	0.0%	0.0%
sodium phenoxyacetate hemihydrate	608-031-7	27006-83-3	27006833	2492	Reach_4259	588	2.68	1.01	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
620-019-3	607-957-9	26567-10-2	26567102	2477	Reach_4255	589	2.94	0.14	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
metformin hydrochloride	238-056-5	14205-39-1	14205391	1944	Reach_2358	590	3.70	0.51	3				-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
sodium N-methyltaurinate	922-576-0	1184182-45-3	1184182453	5617	Reach_5095	591							-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
hydrogen cyanide	200-821-6	74-90-8	74908	841	Reach_116	592	2.72	0.88	12	1.72	0.63	36	-5.0	-4.7	-6.3	0.0%	0.0%	0.0%
609-368-2	618-106-6	88046-01-9	88046019	6074	Reach_4485	593							-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
tert-butylhydrazine monohydrochloride	205-533-4	142-30-3	142303	1953	Reach_1177	594							-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
sulphur dichloride	251-020-3	32388-55-9	32388559	2651	Reach_2661	595	3.27	0.25	3	2.27	0.25		-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
1,2-dichloro-4-nitrobenzene	213-709-7	1003-52-7	1003527	1302	Reach_1634	596	5.66	0.30	3	4.66	0.30		-4.9	-4.7	-5.7	0.0%	0.0%	0.0%
dec-1-ene	212-819-2	872-05-9	872059	3921	Reach_1578	597	3.32	1.28	3	3.84	2.11		-4.9	-4.7	-7.0	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
1,1'-isopropylidenebis(p-phenyleneoxy)dipropan-2-ol	204-137-9	116-37-0	116370	1648	Reach_954	598	4.02	0.31	3	3.02	0.31		-4.1	-4.7	-6.1	0.0%	0.0%	0.0%
didecyldimethylammonium chloride	230-525-2	7173-51-5	7173515	1233	Reach_2228	599	2.42	0.67	22	1.60	0.73	11	-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
hydroquinone	204-617-8	123-31-9	123319	388	Reach_1045	600	2.45	0.68	12	1.45	0.68	24	-4.0	-4.7	-6.3	0.0%	0.0%	0.0%
6-chloro-N,N,N',N'-tetrabutyl-1,3,5-triazine-2,4-diamine	609-724-7	39605-45-3	39605453	2843	Reach_4309	601	0.54	1.12	3				-4.3	-4.7	-6.0	0.0%	0.0%	0.0%
4'-chloro-2-nitrobiphenyl	242-262-0	18379-25-4	18379254	2187	Reach_2460	602	4.83	1.10	3	3.83	1.10		-4.9	-4.7	-5.9	0.0%	0.0%	0.0%
potassium isopentyl dithiocarbonate	213-180-2	928-70-1	928701	6083	Reach_1601	603	3.85	1.06	3	2.85	1.06		-4.4	-4.7	-6.0	0.0%	0.0%	0.0%
cystine	200-296-3	56-89-3	56893	717	Reach_33	604	5.50		4	4.50			-3.8	-4.7	-6.2	0.0%	0.0%	0.0%
bis(2-ethylhexyl) adipate	203-090-1	103-23-1	103231	160	Reach_603	605	3.50	1.35	7	2.50	1.35		-4.5	-4.7	-5.5	0.0%	0.0%	0.0%
thiourea	200-543-5	62-56-6	62566	767	Reach_66	606	4.51	1.43	5	4.14	1.73		-4.2	-4.7	-5.5	0.0%	0.0%	0.0%
tosyl chloride	202-684-8	98-59-9	98599	4188	Reach_514	607	4.57	0.43	3	3.57	0.43		-4.9	-4.7	-6.1	0.0%	0.0%	0.0%
9-hydroxyandrost-4-ene-3,17-dione	202-440-0	95-68-1	95681	1036	Reach_437	608	4.54	0.73	12	3.54	0.73		-3.9	-4.7	-6.3	0.0%	0.0%	0.0%
2,3-didehydro-3-O-sodio-D-erythro-hexono-1,4-lactone	228-973-9	6381-77-7	6381777	5964	Reach_2175	609	5.26	0.25	3	4.26	0.25		-4.5	-4.7	-6.1	0.0%	0.0%	0.0%
disodium aniline-2,5-disulphonate	255-250-5	41184-20-7	41184207	5877	Reach_2737	610							-4.5	-4.7	-6.1	0.0%	0.0%	0.0%
O,O-dimethyl hydrogen dithiophosphate	212-053-9	756-80-9	756809	864	Reach_1527	611	4.67	0.69	4	3.67	0.69		-4.9	-4.7	-5.7	0.0%	0.0%	0.0%
2,5-dichlorophenol	209-520-4	583-78-8	583788	728	Reach_1383	612	3.50	0.84	20	2.50	0.84		-4.9	-4.7	-5.5	0.0%	0.0%	0.0%
2-(2-(2-ethoxyethoxy)ethoxy)ethanol	203-978-9	112-50-5	112505	331	Reach_910	613	7.21	0.89	4	6.21	0.89		-3.9	-4.7	-6.4	0.0%	0.0%	0.0%
imidazolidine-2-thione	202-506-9	96-45-7	96457	1054	Reach_464	614	5.79	1.22	8	4.79	1.22		-4.3	-4.7	-5.5	0.0%	0.0%	0.0%
m-phenoxybenzaldehyde	254-487-1	39515-51-0	39515510	625	Reach_2726	615	3.80	1.18	7	2.80	1.18		-4.9	-4.7	-5.8	0.0%	0.0%	0.0%
1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic a	230-991-7	7397-62-8	7397628	3630	Reach_2247	616	5.23	0.55	3	4.23	0.55		-4.9	-4.7	-5.7	0.0%	0.0%	0.0%
hex-1-ene	209-753-1	592-41-6	592416	3270	Reach_1392	617	3.32	1.28	3	3.84	2.11		-5.0	-4.7	-7.2	0.0%	0.0%	0.0%
1,2-benzisothiazol-3(2H)-one 1,1-dioxide, sodium salt	204-886-1	128-44-9	128449	1189	Reach_1111	618	6.07	0.89	5	5.07	0.89		-4.5	-4.7	-6.1	0.0%	0.0%	0.0%
sodium ethanolate	205-487-5	141-52-6	141526	5691	Reach_1163	619	6.39	0.82	4	5.19	0.97		-4.5	-4.7	-6.1	0.0%	0.0%	0.0%
4-isopropylaniline	247-119-6	25586-42-9	25586429	2439	Reach_2570	620	1.95	0.27	3				-4.9	-4.7	-6.3	0.0%	0.0%	0.0%
690-526-2	690-526-2	38632-47-2	38632472	5870	Reach_4657	621	4.11	0.99	3	3.11	0.99		-4.5	-4.7	-6.1	0.0%	0.0%	0.0%
1,2,3-trichloropropane	202-486-1	96-18-4	96184	1047	Reach_453	622	4.65	0.70	20	3.53	0.70		-5.0	-4.7	-6.1	0.0%	0.0%	0.0%
diethyl phthalate	201-550-6	84-66-2	84662	961	Reach_288	623	4.51	0.72	60	3.99	0.35		-4.9	-4.7	-6.2	0.0%	0.0%	0.0%
triclosan	222-182-2	3380-34-5	3380345	48	Reach_1954	624	2.05	1.03	19	1.42	0.72	10	-4.9	-4.7	-5.5	0.0%	0.0%	0.0%
sodium ascorbate	229-352-5	6485-40-1	6485401	781	Reach_2189	625	4.78	0.66	6	3.78	0.66		-4.5	-4.7	-6.1	0.0%	0.0%	0.0%
2,2,2',2'-tetrakis(hydroxymethyl)-3,3'-oxydipropan-1-ol	204-794-1	126-58-9	126589	1808	Reach_1087	626	6.55		1				-3.8	-4.7	-6.5	0.0%	0.0%	0.0%
1-chloro-2,5-dimethoxy-4-nitrobenzene	230-086-7	6940-53-0	6940530	3543	Reach_2214	627	4.48	0.44	3	3.48	0.44		-4.9	-4.7	-6.3	0.0%	0.0%	0.0%
acetophenone	202-708-7	98-86-2	98862	1077	Reach_521	628	5.18	0.70	16	4.18	0.70		-4.9	-4.7	-5.9	0.0%	0.0%	0.0%
3-nitrotoluene	221-259-8	3048-64-4	3048644	2599	Reach_1906	629	3.80	0.22	3	2.80	0.22		-5.0	-4.7	-5.8	0.0%	0.0%	0.0%
hexan-6-olide	207-938-1	502-44-3	502443	2999	Reach_1300	630	5.75	0.39	3	4.80	0.15		-4.9	-4.7	-6.3	0.0%	0.0%	0.0%
604-340-6	604-340-6	143230-42-6	143230426	1960	Reach_4148	631	3.58	1.28	3				-4.0	-4.7	-6.4	0.0%	0.0%	0.0%
4,6-dichloro-5-nitro-2-(propylthio)pyrimidine	203-679-3	109-54-6	109546	1502	Reach_776	632	3.90	0.76	3				-4.8	-4.7	-6.2	0.0%	0.0%	0.0%
2,3,5,6-tetrachloropyridine	219-283-9	2402-79-1	2402791	2367	Reach_1796	633	3.49	0.44	3	2.59	0.50		-5.0	-4.7	-5.8	0.0%	0.0%	0.0%
acetylene	200-816-9	74-86-2	74862	3649	Reach_112	634	5.29	0.50	3	4.29	0.50		-5.1	-4.7	-6.8	0.0%	0.0%	0.0%
1,3,5-triazine-2,4,6-triyltrinitrilohexamethanol	208-503-9	531-18-0	531180	3088	Reach_1328	635	7.69	0.86	3				-3.9	-4.7	-6.0	0.0%	0.0%	0.0%
tert-butylamine	200-888-1	75-64-9	75649	862	Reach_155	636	4.76	0.53	6	3.76	0.53		-5.0	-4.7	-5.9	0.0%	0.0%	0.0%
tert-butyl [(4R,6R)-6-{2-[2-(4-fluorophenyl)-3-phenyl-4-(phenylca	700-258-0	125971-95-1	125971951	1801	Reach_4827	637	5.50		3	4.50			-4.2	-4.7	-6.1	0.0%	0.0%	0.0%
629-764-9	629-764-9	164524-02-1	164524021	5732	Reach_4596	638	5.50	0.70	3	4.50	0.70		-4.5	-4.7	-6.1	0.0%	0.0%	0.0%
616-280-8	616-280-8	760108-96-1	760108961	6030	Reach_4429	639							-4.5	-4.8	-6.1	0.0%	0.0%	0.0%
tetramethylammonium hydroxide	200-882-9	75-59-2	75592	6027	Reach_153	640	4.69	1.09	3	3.69	1.09		-4.5	-4.8	-6.1	0.0%	0.0%	0.0%
methylamine	200-820-0	74-89-5	74895	840	Reach_115	641	5.22	0.87	7	3.91	0.70		-5.1	-4.8	-5.7	0.0%	0.0%	0.0%
dodecanedioic acid, compound with hexane-1,6-diamine (1:1)	235-697-2	12542-30-2	12542302	1797	Reach_2314	642	3.67	0.28	3	2.67	0.28		-4.5	-4.8	-6.1	0.0%	0.0%	0.0%
4,4'-methylenedicyclohexyl diisocyanate	225-863-2	5124-30-1	5124301	3030	Reach_2079	643	3.87	0.63	3	2.87	0.63		-4.7	-4.8	-5.9	0.0%	0.0%	0.0%
[(2R*, 4R*) -2-(bromomethyl)-2-(2,4-dichlorophenyl)-1,3-dioxola	222-697-2	3577-63-7	3577637	2748	Reach_1974	644	4.63	1.05	3				-4.2	-4.8	-6.0	0.0%	0.0%	0.0%
disodium 4,4'-bis[[4-anilino-6-[(2-carbamoylethyl)(2-hydroxyeth	248-420-5	27344-06-5	27344065	5809	Reach_2601	645	5.34	0.65	3	4.34	0.65		-4.5	-4.8	-6.1	0.0%	0.0%	0.0%
3-nitrobenzaldehyde	210-415-0	615-20-3	615203	3338	Reach_1426	646	3.79	0.15	3	3.06	0.17		-5.0	-4.8	-5.9	0.0%	0.0%	0.0%
2,4-xylidine	611-349-9	560-62-3	560623	3185	Reach_4357	647	4.52	0.55	3				-4.9	-4.8	-6.2	0.0%	0.0%	0.0%
α-chlorotoluene	202-853-6	100-44-7	100447	126	Reach_558	648	3.79	0.70	40	3.15	0.70		-5.0	-4.8	-6.1	0.0%	0.0%	0.0%
methanethiol	200-822-1	74-93-1	74931	3652	Reach_117	649	3.58	0.39	3	2.58	0.39		-5.1	-4.8	-6.5	0.0%	0.0%	0.0%
603-525-9	603-525-9	131860-97-4	131860974	1852	Reach_4123	650	3.00	1.31	3				-4.1	-4.8	-6.4	0.0%	0.0%	0.0%
1,4-dichlorobenzene	203-400-5	106-46-7	106467	192	Reach_668	651	3.74	0.83	25	2.91	0.53	9	-5.0	-4.8	-6.3	0.0%	0.0%	0.0%
androst-4-ene-3,17-dione	200-554-5	63-05-8	63058	75	Reach_67	652	4.14	0.26	3	3.14	0.26		-4.7	-4.8	-6.3	0.0%	0.0%	0.0%
5-amino-1,3-dihydro-2H-benzimidazol-2-one	202-401-8	95-23-8	95238	4123	Reach_424	653	4.75		1				-4.0	-4.8	-6.3	0.0%	0.0%	0.0%
4-nitrotoluene-2-sulphonic acid	204-445-3	121-03-9	121039	1722	Reach_1007	654	5.10		2	4.23			-3.9	-4.8	-6.7	0.0%	0.0%	0.0%
4-nitrobenzoic acid	200-526-2	62-23-7	62237	761	Reach_62	655	5.29	0.70	8	4.29	0.70		-4.3	-4.8	-6.2	0.0%	0.0%	0.0%
cyclohexane-1,2-dicarboxylic anhydride	201-604-9	85-42-7	85427	3889	Reach_295	656	5.90	0.49	3	4.90	0.49		-5.0	-4.8	-6.2	0.0%	0.0%	0.0%
aluminium trilactate	242-670-9	18917-91-4	18917914	5751	Reach_2471	657	3.45	1.28	3	2.45	1.28		-4.5	-4.8	-6.1	0.0%	0.0%	0.0%
tetramethylthiuram monosulphide	202-605-7	97-74-5	97745	1059	Reach_486	658	3.20	0.80	6	1.34	0.29		-4.8	-4.8	-5.8	0.0%	0.0%	0.0%
caffeine	202-078-3	91-57-6	91576	1007	Reach_376	659	3.12	0.70	24	2.12	0.70		-4.2	-4.8	-5.6	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
ziram (reach)	205-288-3	137-30-4	137304	6353	Pest_436	660	2.55	0.75	20	1.86	0.69	9	-4.5	-4.8	-6.1	0.0%	0.0%	0.0%
fluorouracil	228-761-6	6358-08-3	6358083	1283	Reach_2166	661	3.76	0.53	3				-4.0	-4.8	-6.3	0.0%	0.0%	0.0%
flumetasone	639-824-6	1229457-94-6	1229457946	1759	Reach_4607	662	4.07	0.62	3				-4.3	-4.8	-6.0	0.0%	0.0%	0.0%
1,2,3,6-tetrahydrophthalic anhydride	201-605-4	85-43-8	85438	3890	Reach_296	663	5.36	0.30	3	4.36	0.30		-5.0	-4.8	-6.4	0.0%	0.0%	0.0%
acetaldehyde	200-836-8	75-07-0	75070	848	Reach_127	664	4.95	0.82	10	3.95	0.82		-5.0	-4.8	-6.1	0.0%	0.0%	0.0%
octadecyl methacrylate	251-013-5	32360-05-7	32360057	2649	Reach_2660	665	0.57	1.27	3	0.76			-4.8	-4.8	-5.8	0.0%	0.0%	0.0%
malononitrile	203-703-2	109-77-3	109773	266	Reach_791	666	3.02	0.25	5	2.02	0.25		-4.9	-4.8	-6.3	0.0%	0.0%	0.0%
strontium 4-[(5-chloro-4-methyl-2-sulphonatophenyl)azo]-3-hyd	239-879-2	15782-05-5	15782055	5724	Reach_2397	667	4.99	0.82	3	3.99	0.82		-4.5	-4.8	-6.2	0.0%	0.0%	0.0%
hexane-1,6-diaminium benzene-1,4-dicarboxylate	700-230-8	3160-86-9	3160869	5840	Reach_4813	668							-4.6	-4.8	-6.2	0.0%	0.0%	0.0%
688-329-1	688-329-1	10175-31-2	10175312	1327	Reach_4643	669	4.14		2				-5.0	-4.8	-5.9	0.0%	0.0%	0.0%
N-methyldidecylamine	230-990-1	7396-58-9	7396589	3629	Reach_2246	670	1.65	1.25	3	0.62	1.25		-4.7	-4.8	-6.1	0.0%	0.0%	0.0%
trimethyl borate	204-468-9	121-43-7	121437	1726	Reach_1012	671	5.22	0.63	3	4.11	0.48		-4.9	-4.8	-6.5	0.0%	0.0%	0.0%
sodium hydrogen-5-sulphoisophthalate	228-845-2	6362-79-4	6362794	5962	Reach_2173	672							-4.6	-4.8	-6.2	0.0%	0.0%	0.0%
disulfiram	202-607-8	97-77-8	97778	1060	Reach_487	673	2.35	0.78	6	1.26	0.65		-4.7	-4.8	-5.8	0.0%	0.0%	0.0%
potassium sodium 4,4'-bis[6-anilino-4-[bis(2-hydroxyethyl)aminc	275-031-8	70942-01-7	70942017	6007	Reach_2923	674	5.60		1	4.16			-4.5	-4.8	-6.2	0.0%	0.0%	0.0%
benzyltrimethylammonium chloride	200-300-3	56-93-9	56939	1222	Reach_34	675	3.96		2				-4.6	-4.8	-6.2	0.0%	0.0%	0.0%
3,6,9,12-tetraoxotridecanol	245-883-5	23783-42-8	23783428	2359	Reach_2535	676	7.45	0.61	3	6.25	0.65		-4.0	-4.8	-6.6	0.0%	0.0%	0.0%
methylphosphonic acid, compound with amidinourea (1:1)	282-758-4	84402-58-4	84402584	6051	Reach_2972	677	5.51	0.64	3	4.60	1.02		-4.6	-4.8	-6.2	0.0%	0.0%	0.0%
trimethylamine	200-875-0	75-50-3	75503	859	Reach_147	678	5.45	0.58	4	4.32	0.58		-5.1	-4.8	-6.1	0.0%	0.0%	0.0%
sodium hydrogen [N,N-bis[2-[bis(carboxymethyl)amino]ethyl]gly	235-627-0	12389-75-2	12389752	5635	Reach_2313	679	5.34	1.09	3	5.19	0.33		-4.6	-4.8	-6.2	0.0%	0.0%	0.0%
biphenyl-2-ol	201-993-5	90-43-7	90437	106	Reach_364	680	3.45	0.80	27	2.59	0.80		-5.0	-4.8	-6.3	0.0%	0.0%	0.0%
cholic acid	201-337-8	81-25-4	81254	100	Reach_274	681	5.37	0.22	3	4.37	0.22		-4.4	-4.8	-6.3	0.0%	0.0%	0.0%
chlorobenzene	203-628-5	108-90-7	108907	248	Reach_761	682	4.17	0.74	22	3.57	0.69	6	-5.1	-4.8	-6.8	0.0%	0.0%	0.0%
601-639-3	218-817-8	2243-62-1	2243621	542	Reach_1779	683	4.04	0.82	4	2.71	1.24		-5.0	-4.8	-6.3	0.0%	0.0%	0.0%
sulfapyridine	205-642-7	144-83-2	144832	29	Reach_1196	684	4.32	1.03	3	3.32	1.03		-4.4	-4.8	-5.6	0.0%	0.0%	0.0%
isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-diol	246-771-9	25265-77-4	25265774	2426	Reach_2563	685	4.60	0.48	3	3.49	0.41		-5.0	-4.8	-6.4	0.0%	0.0%	0.0%
triisobutyl phosphate	204-798-3	126-71-6	126716	18	Reach_1088	686	4.51	1.01	30	3.74	1.01		-5.1	-4.8	-5.8	0.0%	0.0%	0.0%
2-(ethylthio)ethanol	203-802-0	110-77-0	110770	283	Reach_828	687	4.81	0.59	3	3.81	0.59		-5.1	-4.8	-5.8	0.0%	0.0%	0.0%
guanidinium phosphate (1:1)	226-551-9	5423-22-3	5423223	5924	Reach_2110	688	4.80		1				-4.6	-4.8	-6.2	0.0%	0.0%	0.0%
morpholinium toluene-4-sulphonate	237-301-3	13732-62-2	13732622	5681	Reach_2346	689	5.24	0.49	3	4.24	0.49		-4.6	-4.8	-6.2	0.0%	0.0%	0.0%
2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2-meth	226-789-3	5468-75-7	5468757	3152	Reach_2118	690	5.26	1.21	3	4.26	1.21		-4.6	-4.8	-6.4	0.0%	0.0%	0.0%
hexasodium 2,2'-[vinylenebis[(3-sulphonato-4,1-phenylene)imin	255-217-5	41098-56-0	41098560	5875	Reach_2735	691	5.38	0.59	3	4.38	0.59		-4.6	-4.8	-6.2	0.0%	0.0%	0.0%
2-ethylhexyl palmitate	249-862-1	29806-73-3	29806733	2572	Reach_2631	692	6.29	0.94	3	5.29	0.94		-4.9	-4.8	-5.5	0.0%	0.0%	0.0%
3,7,11,15-tetramethylhexadec-1-en-3-ol	208-008-8	505-32-8	505328	3007	Reach_1307	693	2.21		1				-4.7	-4.8	-5.6	0.0%	0.0%	0.0%
2,6-diisopropylaniline	246-305-4	24544-04-5	24544045	560	Reach_2548	694	4.18		2				-5.1	-4.8	-5.6	0.0%	0.0%	0.0%
2-methyl-p-phenylenediamine sulfate	210-431-8	615-50-9	615509	5951	Reach_1427	695	3.06	0.48	3	2.06	0.48		-4.6	-4.8	-6.2	0.0%	0.0%	0.0%
sodium calcium edetate	200-529-9	62-33-9	62339	5957	Reach_63	696	5.46	0.73	3	4.43	0.84		-4.6	-4.8	-6.2	0.0%	0.0%	0.0%
tris(2-hydroxyethyl)-1,3,5-triazinetrione	212-660-9	839-90-7	839907	3854	Reach_1564	697	6.01	1.92	3	5.00			-4.0	-4.8	-6.4	0.0%	0.0%	0.0%
calcium bis[4-[[1-[[(2-methylphenyl)amino]carbonyl]-2-oxopropy	235-558-6	12286-66-7	12286667	5632	Reach_2312	698	3.69	1.39	3	2.69	1.39		-4.6	-4.8	-6.2	0.0%	0.0%	0.0%
linalool	201-134-4	78-70-6	78706	899	Reach_205	699	4.67	0.27	5	3.99	0.50		-5.1	-4.8	-5.9	0.0%	0.0%	0.0%
2-phenyl-1H-benzimidazole-5-sulphonic acid	248-502-0	27503-81-7	27503817	42	Reach_2608	700	3.79	0.96	3				-4.2	-4.8	-5.6	0.0%	0.0%	0.0%
sodium 1,4-diisodecyl sulphonatosuccinate	249-894-6	29857-13-4	29857134	5826	Reach_2633	701	3.66	0.83	3	2.66	0.83		-4.6	-4.8	-6.2	0.0%	0.0%	0.0%
fumaric acid	203-743-0	110-17-8	110178	276	Reach_807	702	5.33		2				-3.9	-4.8	-6.5	0.0%	0.0%	0.0%
sodium salicylate	200-198-0	54-21-7	54217	1219	Reach_22	703	6.13	0.50	4	3.72	1.03		-4.6	-4.8	-6.2	0.0%	0.0%	0.0%
norflurane	212-377-0	811-97-2	811972	3803	Reach_1549	704	5.60	0.27	3	4.60	0.27		-5.3	-4.8	-7.1	0.0%	0.0%	0.0%
prednisolone	200-021-7	50-24-8	50248	656	Reach_6	705	4.30	1.42	3	3.30	1.42		-4.3	-4.8	-6.1	0.0%	0.0%	0.0%
m-cresol	203-577-9	108-39-4	108394	237	Reach_743	706	4.46	0.84	40	3.41	0.75		-5.0	-4.8	-6.4	0.0%	0.0%	0.0%
hesperidin	208-288-1	520-26-3	520263	3051	Reach_1322	707	5.80	1.88	3				-3.9	-4.8	-6.6	0.0%	0.0%	0.0%
(±)-2-(6-methoxy-2-naphthyl)propionic acid	247-485-7	26159-31-9	26159319	572	Reach_2575	708	5.17	0.10	3	4.17	0.10		-4.7	-4.8	-5.7	0.0%	0.0%	0.0%
N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxobutyramide	247-820-7	26576-46-5	26576465	2478	Reach_2588	709	4.67	1.33	3				-4.0	-4.8	-6.4	0.0%	0.0%	0.0%
dimethyl disulphide	210-871-0	624-92-0	624920	764	Reach_1456	710	3.65	0.58	13	2.79	0.64	13	-5.1	-4.9	-6.3	0.0%	0.0%	0.0%
sodium 2-methylprop-2-ene-1-sulphonate	216-341-5	1561-92-8	1561928	5718	Reach_1691	711							-4.6	-4.9	-6.2	0.0%	0.0%	0.0%
potassium O-pentyl dithiocarbonate	220-329-5	2720-73-2	2720732	1211	Reach_1858	712	4.18	0.62	5	4.03	0.76		-4.6	-4.9	-6.2	0.0%	0.0%	0.0%
dipotassium adipate	242-838-1	19147-16-1	19147161	5754	Reach_2474	713	4.93	0.38	3	3.93	0.38		-4.6	-4.9	-6.2	0.0%	0.0%	0.0%
2,2-bis(chloromethyl)trimethylene bis(bis(2-chloroethyl)phospha	253-760-2	38051-10-4	38051104	2812	Reach_2714	714	4.58	0.36	3	3.75	0.37		-4.9	-4.9	-6.3	0.0%	0.0%	0.0%
oxalic acid	205-634-3	144-62-7	144627	472	Reach_1195	715	5.83	0.69	5	4.83	0.69		-3.9	-4.9	-6.5	0.0%	0.0%	0.0%
acrylaldehyde	203-453-4	107-02-8	107028	205	Reach_690	716	1.97	0.59	29	1.36	0.74	10	-5.1	-4.9	-6.2	0.0%	0.0%	0.0%
carbonic acid, compound with 2-aminoethanol (1:2)	244-600-2	21829-52-7	21829527	5775	Reach_2510	717	4.72	0.59	3	3.72	0.59		-4.6	-4.9	-6.2	0.0%	0.0%	0.0%
2,4-dinitrophenol	200-087-7	51-28-5	51285	57	Reach_14	718	3.92	0.74	31	2.65	0.64	9	-4.4	-4.9	-5.6	0.0%	0.0%	0.0%
D-gluconic acid	208-401-4	526-95-4	526954	3069	Reach_1324	719	6.00		1				-3.8	-4.9	-6.5	0.0%	0.0%	0.0%
calcium(2+) 12-hydroxyoctadecanoate	221-605-8	3159-62-4	3159624	5839	Reach_1922	720	5.74	1.14	3	4.74	1.14		-4.6	-4.9	-6.2	0.0%	0.0%	0.0%
trichloroacetic acid	200-927-2	76-03-9	76039	90	Reach_170	721	5.65	1.16	22	3.63	2.26	3	-4.4	-4.9	-6.0	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
xylose	200-400-7	58-86-6	58866	3256	Reach_49	722	8.11		1				-4.0	-4.9	-6.6	0.0%	0.0%	0.0%
1-(7-bromo-9,9-difluoro-9H-fluoren-2-yl)-2-chloroethanone	203-483-8	107-35-7	107357	1460	Reach_705	723	5.38	1.11	3				-4.0	-4.9	-6.4	0.0%	0.0%	0.0%
terephthaloyl dichloride	202-829-5	100-20-9	100209	1297	Reach_551	724	6.30	0.30	3	5.30	0.30		-5.1	-4.9	-6.4	0.0%	0.0%	0.0%
diammonium [N,N-bis[2-[bis(carboxymethyl)amino]ethyl]glycina	289-064-0	85959-68-8	85959688	6062	Reach_2988	725	5.34	1.09	3	5.19	0.33		-4.6	-4.9	-6.2	0.0%	0.0%	0.0%
triphenyl phosphate	233-713-2	10326-41-7	10326417	161	Reach_2288	726	5.75	0.50	3	5.14	0.48		-4.9	-4.9	-6.3	0.0%	0.0%	0.0%
dimethyl ether	204-065-8	115-10-6	115106	1630	Reach_936	727	5.77	0.54	3	4.77	0.54		-5.2	-4.9	-6.3	0.0%	0.0%	0.0%
(3-chloropropyl)triethoxysilane	225-805-6	5089-70-3	5089703	3022	Reach_2077	728	5.31	0.86	3	4.31	0.86		-5.1	-4.9	-6.0	0.0%	0.0%	0.0%
aspartic acid	200-291-6	56-84-8	56848	3212	Reach_31	729	5.37	0.97	3	4.18	0.46		-3.8	-4.9	-6.6	0.0%	0.0%	0.0%
n-hexane	203-777-6	110-54-3	110543	279	Reach_817	730	4.96	0.78	14	3.96	0.70	56	-5.1	-4.9	-7.4	0.0%	0.0%	0.0%
4-(2-hydroxypropan-2-yl)-2-propyl-1-{[2'-(1H-tetrazol-5-yl)biphe	209-057-8	554-00-7	554007	700	Reach_1362	731	3.69	0.62	19	2.11	0.71	4	-4.4	-4.9	-6.4	0.0%	0.0%	0.0%
sodium hydrogen [6R-(6α,7β)]-3-(acetoxymethyl)-7-[(5-amino-5-	203-227-5	104-68-7	104687	1399	Reach_627	732	5.70	0.20	3	4.70	0.20		-4.6	-4.9	-6.2	0.0%	0.0%	0.0%
triethylamine	204-469-4	121-44-8	121448	370	Reach_1013	733	4.83	0.63	5	4.19	0.59		-5.1	-4.9	-6.2	0.0%	0.0%	0.0%
2-ethylhexanal	204-596-5	123-05-7	123057	1761	Reach_1038	734	3.73	0.23	3	2.72	0.29		-5.1	-4.9	-6.4	0.0%	0.0%	0.0%
6H-dibenz[c,e][1,2]oxaphosphorin 6-oxide	252-813-7	35948-25-5	35948255	2754	Reach_2696	735	5.14	0.57	3	4.14	0.57		-4.8	-4.9	-6.4	0.0%	0.0%	0.0%
pyrocatechol	204-427-5	120-80-9	120809	361	Reach_1002	736	4.00	0.47	5	3.45	0.35		-4.3	-4.9	-6.5	0.0%	0.0%	0.0%
4-chlorobenzenesulphonyl chloride	200-870-3	75-44-5	75445	3672	Reach_144	737	4.83	0.59	3				-5.1	-4.9	-6.1	0.0%	0.0%	0.0%
2'-methoxyacetoacetanilide	202-131-0	92-15-9	92159	4029	Reach_383	738	5.59		1				-4.1	-4.9	-6.6	0.0%	0.0%	0.0%
3-methylbut-3-en-1-ol	212-110-8	763-32-6	763326	3709	Reach_1536	739	5.97	0.37	3	4.97	0.37		-5.1	-4.9	-6.1	0.0%	0.0%	0.0%
[(butoxymethylethoxy)methylethoxy]propan-1-ol	259-910-3	55934-93-5	55934935	3182	Reach_2811	740	5.69	0.62	3	4.69	0.62		-4.8	-4.9	-6.5	0.0%	0.0%	0.0%
proxan-sodium	205-443-5	140-93-2	140932	1197	Reach_1154	741	4.16	0.91	5	4.63	0.94		-4.6	-4.9	-6.2	0.0%	0.0%	0.0%
(E)-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	201-224-3	79-77-6	79776	926	Reach_249	742	3.85	0.32	4	3.02	0.34		-5.1	-4.9	-5.9	0.0%	0.0%	0.0%
2-chloropropionic acid	209-952-3	598-78-7	598787	3293	Reach_1406	743	4.91		2				-4.0	-4.9	-6.5	0.0%	0.0%	0.0%
4,4'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[2,4-dihydr	239-898-6	15793-73-4	15793734	2057	Reach_2399	744	1.09	0.57	3	3.00			-4.4	-4.9	-6.0	0.0%	0.0%	0.0%
perylene-3,4:9,10-tetracarboxydiimide	201-344-6	81-33-4	81334	3804	Reach_275	745	5.13	2.03	3	4.13	2.03		-4.3	-4.9	-6.2	0.0%	0.0%	0.0%
dichlobenil (reach)	214-787-5	1194-65-6	1194656	352	Reach_1672	746	3.97	0.58	51	2.55	0.76	10	-5.1	-4.9	-5.7	0.0%	0.0%	0.0%
N,N-diethylaniline	202-088-8	91-66-7	91667	1009	Reach_378	747	4.04	0.50	5	3.04	0.70		-5.1	-4.9	-5.7	0.0%	0.0%	0.0%
tetrakis(hydroxymethyl)phosphonium sulphate(2:1)	259-709-0	55566-30-8	55566308	1221	Reach_2809	748	4.54	0.57	5	3.51	0.60		-4.6	-4.9	-6.2	0.0%	0.0%	0.0%
4-(2-aminoethyl)benzenesulphonamide	252-501-0	35303-76-5	35303765	2729	Reach_2688	749	4.88	0.95	3				-4.2	-4.9	-6.5	0.0%	0.0%	0.0%
sodium diisobutylnaphthalenesulphonate	248-326-4	27213-90-7	27213907	5808	Reach_2598	750	5.08	0.16	3	4.08	0.16		-4.6	-4.9	-6.2	0.0%	0.0%	0.0%
trichloro(3-chloropropyl)silane	219-844-8	2550-06-3	2550063	1251	Reach_1837	751	5.93	0.39	3	4.93	0.39		-5.1	-4.9	-6.0	0.0%	0.0%	0.0%
octan-1-ol	203-917-6	111-87-5	111875	314	Reach_878	752	4.50	0.70	60	3.10	0.37		-5.1	-4.9	-6.2	0.0%	0.0%	0.0%
8,18-dichloro-5,15-diethyl-5,15-dihydrodiindolo[3,2-b:3',2'-m]tri	228-767-9	6358-30-1	6358301	3406	Reach_2167	753	5.32	0.49	3	4.32	0.49		-4.9	-4.9	-5.4	0.0%	0.0%	0.0%
mycophenolic acid	246-119-3	24280-93-1	24280931	2383	Reach_2541	754	3.70		2				-4.4	-4.9	-6.5	0.0%	0.0%	0.0%
nitrilotriacetonitrile	230-804-9	7327-60-8	7327608	3617	Reach_2237	755							-4.1	-4.9	-6.5	0.0%	0.0%	0.0%
hydrocortisone	200-020-1	50-23-7	50237	655	Reach_5	756	4.88	0.30	3				-4.2	-4.9	-6.3	0.0%	0.0%	0.0%
o-(p-isocyanatobenzyl)phenyl isocyanate	227-534-9	5873-54-1	5873541	3254	Reach_2139	757	5.11		1	4.00			-5.0	-4.9	-6.3	0.0%	0.0%	0.0%
hexadec-1-ene	211-105-8	629-73-2	629732	3391	Reach_1470	758	3.32	1.28	3	3.84	2.09		-4.9	-4.9	-6.6	0.0%	0.0%	0.0%
quinoline	202-051-6	91-22-5	91225	1006	Reach_374	759	4.57	0.49	15	3.42	0.48	4	-5.1	-4.9	-6.1	0.0%	0.0%	0.0%
3-(difluoromethyl)-1-methyl-1H-pyrazole-4-carboxylic acid	204-004-5	112-76-5	112765	1602	Reach_923	760	3.64	1.09	3	2.64	1.09		-4.1	-4.9	-6.6	0.0%	0.0%	0.0%
cyclohexylamine	203-629-0	108-91-8	108918	249	Reach_762	761	4.83	0.70	32	3.69	0.70		-5.1	-4.9	-6.0	0.0%	0.0%	0.0%
2,6-di-tert-butyl-p-cresol	204-881-4	128-37-0	128370	413	Reach_1108	762	3.04	0.84	28	2.10	0.84		-5.1	-4.9	-6.2	0.0%	0.0%	0.0%
cetrimonium chloride	203-928-6	112-02-7	112027	7	Reach_884	763	2.52	0.83	11	1.52	0.83	11	-4.7	-4.9	-6.4	0.0%	0.0%	0.0%
611-255-8	629-377-5	67442-07-3	67442073	3491	Reach_4592	764	4.24	1.87	3				-4.5	-4.9	-6.5	0.0%	0.0%	0.0%
acetonitrile	200-835-2	75-05-8	75058	847	Reach_126	765	5.66	0.72	14	5.52	0.56	4	-5.1	-4.9	-6.0	0.0%	0.0%	0.0%
6-methyl-1,2,3-oxathiazin-4(3H)-one 2,2-dioxide, potassium salt	259-715-3	55589-62-3	55589623	63	Reach_2810	766	6.36		1	5.00			-4.1	-4.9	-6.5	0.0%	0.0%	0.0%
3,5,5-trimethylhexanoic acid	221-975-0	3302-10-1	3302101	1259	Reach_1944	767	4.94	0.20	3	3.94	0.20		-5.1	-4.9	-6.4	0.0%	0.0%	0.0%
propan-1-ol	200-746-9	71-23-8	71238	817	Reach_99	768	6.54	0.70	108	5.53	0.70		-5.1	-4.9	-6.2	0.0%	0.0%	0.0%
tetrabutylammonium bromide	216-699-2	1643-19-2	1643192	1201	Reach_1703	769	5.42	0.66	4	4.42	0.66		-4.7	-4.9	-6.3	0.0%	0.0%	0.0%
azelaic acid	204-669-1	123-99-9	123999	1782	Reach_1064	770	4.05	0.68	3	3.05	0.68		-4.4	-4.9	-6.5	0.0%	0.0%	0.0%
3-aminopropyltriethoxysilane	213-048-4	919-30-2	919302	4023	Reach_1589	771	5.58	0.96	3	4.58	0.96		-5.1	-4.9	-6.5	0.0%	0.0%	0.0%
dibenzoyl peroxide	202-327-6	94-36-0	94360	4103	Reach_414	772	2.48	0.63	3	1.52	0.83		-5.1	-4.9	-6.4	0.0%	0.0%	0.0%
tetrachlorophthalic anhydride	204-171-4	117-08-8	117088	1655	Reach_957	773	5.63	0.51	3	4.63	0.51		-4.9	-4.9	-6.1	0.0%	0.0%	0.0%
α,2-dichlorotoluene	226-009-1	5216-25-1	5216251	3054	Reach_2086	774	4.88		2				-5.2	-4.9	-6.4	0.0%	0.0%	0.0%
3,3',3'',5,5',5''-hexa-tert-butyl-α,α',α''-(mesitylene-2,4,6-triyl)tri-	216-971-0	1709-70-2	1709702	2121	Reach_1711	775	5.03	1.28	3	4.03	1.28		-5.1	-4.9	-3.5	0.0%	0.0%	0.0%
icosan-1-ol	211-119-4	629-96-9	629969	3393	Reach_1472	776	0.49	0.50	3				-4.7	-4.9	-5.7	0.0%	0.0%	0.0%
1,3-bis(hydroxymethyl)-5,5-dimethylimidazolidine-2,4-dione	229-222-8	6440-58-0	6440580	779	Reach_2186	777	5.02	0.93	5	4.21	0.92		-4.1	-4.9	-6.3	0.0%	0.0%	0.0%
m-phenylenediamine	203-584-7	108-45-2	108452	1484	Reach_746	778	4.42	0.98	3	3.42	0.98		-4.1	-4.9	-6.5	0.0%	0.0%	0.0%
2-diphenylphosphinobenzoic acid	623-635-0	27298-98-2	27298982	2498	Reach_4577	779	4.30		2				-4.6	-4.9	-6.5	0.0%	0.0%	0.0%
ephedrine hydrochloride	200-908-9	75-85-4	75854	865	Reach_164	780	6.22	0.70	12	5.27	0.70		-4.7	-4.9	-6.3	0.0%	0.0%	0.0%
sodium 2-[(2-aminoethyl)amino]ethanesulphonate	201-940-6	89-79-2	89792	995	Reach_352	781	5.10		2				-4.7	-4.9	-6.3	0.0%	0.0%	0.0%
sodium 5-oxo-L-prolinate	202-848-9	100-40-3	100403	1305	Reach_555	782	4.23		1				-4.7	-4.9	-6.3	0.0%	0.0%	0.0%
magnesium acrylate	227-177-9	5698-98-6	5698986	5937	Reach_2132	783	4.96	1.31	3	3.96	1.31		-4.7	-4.9	-6.3	0.0%	0.0%	0.0%

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Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
618-804-0	618-804-0	919-94-8	919948	4026	Reach_4500	784	5.31	0.27	3	4.31	0.27		-5.2	-4.9	-6.7	0.0%	0.0%	0.0%
perhydro-1,3,5-trinitro-1,3,5-triazine	204-500-1	121-82-4	121824	375	Reach_1019	785	4.23	0.97	21	3.41	0.47	7	-4.1	-4.9	-6.5	0.0%	0.0%	0.0%
diphenyl ether	202-981-2	101-84-8	101848	150	Reach_584	786	3.29	0.47	7	2.29	0.47		-5.2	-4.9	-6.0	0.0%	0.0%	0.0%
2-chlorobenzamide	210-536-9	617-89-0	617890	3353	Reach_1436	787	4.28	0.83	3				-4.7	-4.9	-6.5	0.0%	0.0%	0.0%
601-672-3	601-672-3	120118-14-1	120118141	1705	Reach_4099	788	2.85		1				-4.4	-4.9	-6.5	0.0%	0.0%	0.0%
benzaldehyde	202-860-4	100-52-7	100527	130	Reach_562	789	4.47	0.65	19	3.79	0.88	3	-5.1	-4.9	-6.1	0.0%	0.0%	0.0%
isobutyrophenone	227-824-5	5994-61-6	5994616	3297	Reach_2149	790	5.20		1				-5.2	-4.9	-6.0	0.0%	0.0%	0.0%
2-chlorobuta-1,3-diene	204-818-0	126-99-8	126998	1810	Reach_1094	791	4.06	0.45	3	3.06	0.45		-5.2	-4.9	-7.2	0.0%	0.0%	0.0%
3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-l	231-710-0	7695-91-2	7695912	3727	Reach_2270	792	5.66	1.01	3	4.66	1.01		-5.1	-4.9	-5.3	0.0%	0.0%	0.0%
4-(chloromethyl)-5-methyl-1,3-dioxol-2-one	251-203-8	32768-54-0	32768540	2661	Reach_2666	793	3.43	0.26	3				-4.4	-4.9	-6.5	0.0%	0.0%	0.0%
choline hydroxide	204-625-1	123-41-1	123411	5634	Reach_1049	794	5.70		1	4.73			-4.7	-4.9	-6.3	0.0%	0.0%	0.0%
sodium mercaptoacetate	206-696-4	367-51-1	367511	5861	Reach_1254	795	5.07	0.89	3	4.07	0.89		-4.7	-4.9	-6.3	0.0%	0.0%	0.0%
2,4-di-tert-butylphenol	202-532-0	96-76-4	96764	4153	Reach_470	796	3.21	0.70	3	2.40	0.79		-5.1	-4.9	-6.3	0.0%	0.0%	0.0%
tetrachloro-p-benzoquinone	204-274-4	118-75-2	118752	1677	Reach_969	797	3.30	0.53	3	2.30	0.53		-4.4	-4.9	-6.2	0.0%	0.0%	0.0%
1,1-dichloroethylene	200-864-0	75-35-4	75354	857	Reach_140	798	5.19	0.49	11	4.03	0.70	12	-5.2	-4.9	-7.1	0.0%	0.0%	0.0%
5,12-dihydro-2,9-dimethylquino[2,3-b]acridine-7,14-dione	213-561-3	980-26-7	980267	4177	Reach_1624	799	5.18	0.72	3	4.18	0.72		-4.3	-4.9	-6.3	0.0%	0.0%	0.0%
L-alanine	200-273-8	56-41-7	56417	3198	Reach_28	800	4.36	1.07	3	3.36	1.07		-3.9	-4.9	-6.7	0.0%	0.0%	0.0%
butyl methacrylate	202-615-1	97-88-1	97881	1061	Reach_490	801	4.93	0.60	4	3.75	0.52		-5.2	-4.9	-6.3	0.0%	0.0%	0.0%
1,1',1'',1'''-ethylenedinitrilotetrapropan-2-ol	203-041-4	102-60-3	102603	1347	Reach_594	802	5.55	1.18	3	4.55	1.18		-4.0	-4.9	-6.7	0.0%	0.0%	0.0%
2-chlorobenzonitrile	212-836-5	873-32-5	873325	3927	Reach_1581	803	4.77	0.15	3	3.77	0.15		-5.2	-4.9	-6.1	0.0%	0.0%	0.0%
L-xylo-hex-2-ulosonic acid	208-403-5	526-98-7	526987	3071	Reach_1325	804	7.77		1				-3.9	-4.9	-6.6	0.0%	0.0%	0.0%
sodium O,O-diisobutyl dithiophosphate	258-508-5	53378-51-1	53378511	5920	Reach_2792	805	5.42		1				-4.7	-4.9	-6.3	0.0%	0.0%	0.0%
4-(α,α-dimethylbenzyl)phenol	209-968-0	599-64-4	599644	3299	Reach_1410	806	3.04	0.10	3	2.04	0.10		-5.1	-4.9	-6.3	0.0%	0.0%	0.0%
612-366-4	612-366-4	6172-80-1	6172801	3350	Reach_4375	807	4.75		1				-5.1	-4.9	-6.3	0.0%	0.0%	0.0%
ethylene di(acetate)	203-881-1	111-55-7	111557	305	Reach_861	808	4.89	0.14	3	3.89	0.14		-5.2	-5.0	-6.4	0.0%	0.0%	0.0%
5,5,5',5'-tetramethyl-2,2'-bi-1,3,2-dioxaborinane	617-343-2	82530-64-1	82530641	3825	Reach_4451	809	3.70		1				-4.4	-5.0	-6.5	0.0%	0.0%	0.0%
calcium sulphidoacetate	249-881-5	29820-13-1	29820131	5825	Reach_2632	810	5.07	0.89	3	4.07	0.89		-4.7	-5.0	-6.3	0.0%	0.0%	0.0%
8-bromo-7-(but-2-yn-1-yl)-3-methyl-3,7-dihydro-1H-purine-2,6-d	203-870-1	111-44-4	111444	301	Reach_857	811	5.58	0.70	16	4.58	0.70		-4.2	-5.0	-6.5	0.0%	0.0%	0.0%
2-methylbut-3-yn-2-ol	204-070-5	115-19-5	115195	339	Reach_939	812	6.03	0.43	4	5.33	0.31		-5.2	-5.0	-5.9	0.0%	0.0%	0.0%
trans-4-aminocyclohexan-1-ol	616-451-7	77326-36-4	77326364	3731	Reach_4439	813	3.97	0.73	3				-5.1	-5.0	-6.3	0.0%	0.0%	0.0%
salicylamide	200-609-3	65-45-2	65452	784	Reach_76	814	4.34	1.14	4	3.33	1.24		-5.2	-5.0	-6.3	0.0%	0.0%	0.0%
potassium tert-butanolate	212-740-3	865-47-4	865474	6065	Reach_1569	815							-4.7	-5.0	-6.3	0.0%	0.0%	0.0%
(6R-trans)-7-amino-3-[[(5-methyl-1,3,4-thiadiazol-2-yl)thio]meth	201-755-0	87-59-2	87592	978	Reach_311	816	4.33	0.84	16	3.33	0.84		-4.0	-5.0	-6.5	0.0%	0.0%	0.0%
N-(2,6-dimethylphenyl)pyridine-2-carboxamide	208-601-1	534-52-1	534521	682	Reach_1332	817	3.11	0.54	12	3.05	0.74	14	-4.4	-5.0	-6.5	0.0%	0.0%	0.0%
(6R-trans)-7-amino-3-chloro-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-	600-558-0	104358-16-9	104358169	1390	Reach_4068	818	2.60	0.09	3				-4.0	-5.0	-6.5	0.0%	0.0%	0.0%
4,6-dichloropyrimidine	224-698-3	4454-05-1	4454051	1269	Reach_2038	819	5.61		1				-5.2	-5.0	-6.1	0.0%	0.0%	0.0%
nicotinic acid	200-441-0	59-67-6	59676	739	Reach_52	820	5.29	0.61	4	4.29	0.61		-4.2	-5.0	-6.6	0.0%	0.0%	0.0%
diallyl 2,2'-oxydiethyl dicarbonate	205-528-7	142-22-3	142223	1951	Reach_1175	821	3.77		2	4.38			-4.9	-5.0	-6.6	0.0%	0.0%	0.0%
Ethyl N-[3-amino-4-(methylamino)benzoyl]-N-pyridin-2-yl-β-alan	203-768-7	110-44-1	110441	1521	Reach_815	822	4.92	0.36	3	4.18	0.51		-4.1	-5.0	-6.6	0.0%	0.0%	0.0%
2-butoxyethyl acetate	203-933-3	112-07-2	112072	1573	Reach_887	823	5.21	0.55	3	4.14	0.65		-5.2	-5.0	-6.2	0.0%	0.0%	0.0%
4-methylpentan-2-one	203-550-1	108-10-1	108101	229	Reach_728	824	6.02	0.39	6	4.94	0.54		-5.2	-5.0	-6.3	0.0%	0.0%	0.0%
2-Chlorodibenzo[b,f][1,4]thiazepin-11(10H)-one	248-492-8	27489-62-9	27489629	576	Reach_2607	825	4.55	0.93	3				-4.6	-5.0	-6.5	0.0%	0.0%	0.0%
4-chlorobenzaldehyde	203-247-4	104-88-1	104881	171	Reach_631	826	3.96	0.47	6	2.96	0.47		-5.2	-5.0	-6.1	0.0%	0.0%	0.0%
propionaldehyde	204-623-0	123-38-6	123386	391	Reach_1047	827	4.86	0.41	5	3.86	0.41		-5.2	-5.0	-6.3	0.0%	0.0%	0.0%
3-chloropropyltrimethoxysilane	219-787-9	2530-87-2	2530872	2430	Reach_1832	828	5.93	0.39	3	4.93	0.39		-5.2	-5.0	-6.1	0.0%	0.0%	0.0%
4-phenylmorpholin-3-one	225-172-6	4698-11-7	4698117	1270	Reach_2056	829	3.34		2				-4.9	-5.0	-6.7	0.0%	0.0%	0.0%
bis(α,α-dimethylbenzyl) peroxide	201-279-3	80-43-3	80433	3791	Reach_262	830	3.43	0.78	3	2.43	0.78		-5.0	-5.0	-6.3	0.0%	0.0%	0.0%
tris(methylphenyl) phosphite	203-446-6	106-95-6	106956	204	Reach_685	831	2.71	0.41	5	1.71	0.41		-4.6	-5.0	-5.6	0.0%	0.0%	0.0%
2-(trifluoromethyl)benzenesulfonamide	700-280-0	1869-24-5	1869245	2205	Reach_4839	832	4.29	1.19	3				-5.1	-5.0	-6.5	0.0%	0.0%	0.0%
disodium 4,4'-dinitrostilbene-2,2'-disulphonate	223-051-2	3709-43-1	3709431	5862	Reach_1985	833	5.17		1				-4.7	-5.0	-6.3	0.0%	0.0%	0.0%
(3-methacrylamidopropyl)trimethylammonium chloride	257-182-1	51410-72-1	51410721	5905	Reach_2773	834	6.28	0.68	3	5.28	0.68		-4.7	-5.0	-6.3	0.0%	0.0%	0.0%
hexan-1-ol	203-852-3	111-27-3	111273	294	Reach_850	835	5.26	0.42	11	4.18	0.40	4	-5.2	-5.0	-6.4	0.0%	0.0%	0.0%
decan-1-ol	203-956-9	112-30-1	112301	325	Reach_896	836	3.66	0.70	36	2.85	0.70		-5.2	-5.0	-6.3	0.0%	0.0%	0.0%
607-864-3	607-864-3	26116-57-4	26116574	5802	Reach_4250	837							-4.7	-5.0	-6.3	0.0%	0.0%	0.0%
2,3-epoxypropyl phenyl ether	204-557-2	122-60-1	122601	381	Reach_1032	838	4.68		2				-5.2	-5.0	-6.1	0.0%	0.0%	0.0%
Bis (acetato-κO)[7-chloro-1-cyclopropyl-6-fluoro-4-(oxo-&#	700-382-5	119618-67-6	119618676	1697	Reach_4883	839							-4.3	-5.0	-6.5	0.0%	0.0%	0.0%
[(±)-(4-amino-2-hydroxy-4-oxobutyl)trimethylammonium] chlori	226-073-0	5261-99-4	5261994	5914	Reach_2088	840							-4.7	-5.0	-6.3	0.0%	0.0%	0.0%
3-aminopropan-1-ol	205-864-4	156-87-6	156876	494	Reach_1216	841	5.25	0.75	6	4.71	0.75		-4.8	-5.0	-6.5	0.0%	0.0%	0.0%
bis(2-methoxyethyl) ether	203-924-4	111-96-6	111966	318	Reach_883	842	6.34	0.53	3	5.74	0.70		-5.2	-5.0	-5.8	0.0%	0.0%	0.0%
2-chloro-N-methoxy-N-methylacetamide	201-141-2	78-77-3	78773	3757	Reach_207	843	4.61	0.26	3				-5.2	-5.0	-6.5	0.0%	0.0%	0.0%
dimantine	204-694-8	124-28-7	124287	1790	Reach_1075	844	2.12	0.66	3	1.18	0.77		-4.9	-5.0	-6.5	0.0%	0.0%	0.0%
potassium hydrogen tartrate	212-769-1	868-14-4	868144	6070	Reach_1573	845	5.86		2				-4.7	-5.0	-6.3	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
tetrafluoroethylene	204-126-9	116-14-3	116143	1645	Reach_951	846	5.19		2				-5.3	-5.0	-7.3	0.0%	0.0%	0.0%
3-(trichlorosilyl)propiononitrile	213-986-4	1071-22-3	1071223	1455	Reach_1640	847	5.19	0.85	3	4.19	0.85		-5.2	-5.0	-6.2	0.0%	0.0%	0.0%
dexpanthenol	201-327-3	81-13-0	81130	3802	Reach_272	848	6.17	1.15	3	5.17	1.15		-4.0	-5.0	-6.6	0.0%	0.0%	0.0%
cyanoacetic acid	206-743-9	372-09-8	372098	2794	Reach_1257	849	4.57	0.61	3	3.72	0.77		-4.1	-5.0	-6.6	0.0%	0.0%	0.0%
diisopropylamine	200-855-1	75-26-3	75263	3660	Reach_135	850	4.98		2	3.89			-5.2	-5.0	-6.4	0.0%	0.0%	0.0%
605-460-1	219-755-4	2524-04-1	2524041	1248	Reach_1829	851	3.94		2				-5.0	-5.0	-6.7	0.0%	0.0%	0.0%
(3H)-benzofuran-2-one	209-052-0	553-86-6	553866	3169	Reach_1361	852	4.31	1.04	3	3.31	1.04		-5.2	-5.0	-6.6	0.0%	0.0%	0.0%
5-chloro-2-phenoxyaniline	204-125-3	116-11-0	116110	1644	Reach_950	853	5.02	0.36	3	4.02	0.36		-4.5	-5.0	-6.5	0.0%	0.0%	0.0%
N-1-naphthylaniline	201-983-0	90-30-2	90302	1002	Reach_362	854	2.89	0.27	5	1.89	0.27		-4.9	-5.0	-5.8	0.0%	0.0%	0.0%
isopulegol	249-277-1	28874-51-3	28874513	5820	Reach_2625	855	4.89		1				-5.2	-5.0	-6.0	0.0%	0.0%	0.0%
2-chloronicotinic acid	220-937-0	2942-59-8	2942598	2566	Reach_1890	856	4.73	0.78	3	3.73	0.78		-4.2	-5.0	-6.7	0.0%	0.0%	0.0%
glyoxal	203-474-9	107-22-2	107222	217	Reach_701	857	5.27	0.34	5	4.52	0.67		-5.2	-5.0	-6.3	0.0%	0.0%	0.0%
2,2'-bipyridyl	206-674-4	366-18-7	366187	2770	Reach_1252	858	4.36	1.03	3				-4.3	-5.0	-6.7	0.0%	0.0%	0.0%
phenothiazine	202-196-5	92-84-2	92842	4051	Reach_394	859	5.01	0.51	3	4.01	0.51		-4.6	-5.0	-6.6	0.0%	0.0%	0.0%
N-(hydroxymethyl)acrylamide	213-103-2	924-42-5	924425	4033	Reach_1593	860	4.91		2	3.42			-3.9	-5.0	-6.7	0.0%	0.0%	0.0%
sodium O,O-diethyl dithiophosphate	222-079-2	3338-24-7	3338247	5847	Reach_1950	861	5.76		2				-4.8	-5.0	-6.4	0.0%	0.0%	0.0%
octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine	220-260-0	2691-41-0	2691410	575	Reach_1855	862	4.48	0.70	48	3.52	0.70		-4.3	-5.0	-6.3	0.0%	0.0%	0.0%
sodium N-chlorobenzenesulphonamide	210-959-9	626-67-5	626675	769	Reach_1458	863	4.62	0.70	12	3.62	0.70		-4.8	-5.0	-6.4	0.0%	0.0%	0.0%
disodium adipate	204-682-2	124-12-9	124129	1785	Reach_1069	864	4.20		1				-4.8	-5.0	-6.4	0.0%	0.0%	0.0%
octanoic acid	204-677-5	124-07-2	124072	401	Reach_1066	865	4.81	0.45	4	3.61	1.67		-5.0	-5.0	-6.6	0.0%	0.0%	0.0%
N-(4-amino-2-ethoxyphenyl)acetamide	203-503-5	107-56-2	107562	1465	Reach_711	866	4.77	0.42	3	3.77	0.42		-4.2	-5.0	-6.5	0.0%	0.0%	0.0%
zinc methacrylate	236-144-8	13189-00-9	13189009	5665	Reach_2327	867	2.84	0.77	3	2.97	1.25		-4.8	-5.0	-6.4	0.0%	0.0%	0.0%
N-(2-methoxy-5-methylphenyl)acetamide	230-157-2	6962-44-3	6962443	3546	Reach_2215	868	3.87	1.04	3				-4.5	-5.0	-6.5	0.0%	0.0%	0.0%
619-874-5	619-874-5	42355-78-2	42355782	1242	Reach_4551	869				4.16			-4.7	-5.0	-6.4	0.0%	0.0%	0.0%
nitrilotriacetic acid	205-355-7	139-13-9	139139	27	Reach_1142	870	5.35	0.38	7	4.05	0.38		-4.3	-5.0	-5.8	0.0%	0.0%	0.0%
chloroacetyl chloride	201-171-6	79-04-9	79049	910	Reach_225	871	3.76	1.69	3	2.76	0.75		-5.3	-5.0	-6.5	0.0%	0.0%	0.0%
1-phenoxypropan-2-ol	212-222-7	770-35-4	770354	3730	Reach_1544	872	5.43	0.52	3	4.43	0.52		-5.2	-5.0	-6.6	0.0%	0.0%	0.0%
sodium N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxyna	217-461-0	1860-26-0	1860260	2200	Reach_1728	873	5.23	1.86	3	4.23	1.86		-4.8	-5.0	-6.4	0.0%	0.0%	0.0%
3-(3-Amino-2-cyanophenoxy)-2,2-dimethyl-N-propylpropanamid	226-467-2	5407-04-5	5407045	1184	Reach_2105	874	5.12		1				-4.5	-5.0	-6.5	0.0%	0.0%	0.0%
2-methylimidazole	211-765-7	693-98-1	693981	806	Reach_1509	875	5.37	0.19	4	4.34	0.61		-4.3	-5.0	-6.6	0.0%	0.0%	0.0%
600-314-3	606-907-3	22038-86-4	22038864	2315	Reach_4224	876	4.72		1				-4.3	-5.0	-6.5	0.0%	0.0%	0.0%
N,N-dimethyldocosylamine	244-433-5	21542-96-1	21542961	2298	Reach_2506	877	2.17	2.15	3	1.17	2.15		-5.1	-5.0	-5.9	0.0%	0.0%	0.0%
1,3,5-triazine-2,4,6(1H,3H,5H)-trithione, trisodium salt	241-749-5	17766-26-6	17766266	5742	Reach_2442	878	5.27	0.62	3	4.27	0.62		-4.8	-5.0	-6.4	0.0%	0.0%	0.0%
6-phenyl-1,3,5-triazine-2,4-diyldiamine	202-095-6	91-76-9	91769	4021	Reach_380	879	4.80	0.22	3	3.80	0.22		-4.3	-5.0	-6.6	0.0%	0.0%	0.0%
603-373-3	601-577-7	118969-29-2	118969292	5619	Reach_4093	880							-4.5	-5.0	-5.9	0.0%	0.0%	0.0%
2-chlorobenzothiazole	222-315-4	3423-28-7	3423287	2697	Reach_1958	881	5.13		1				-4.4	-5.0	-6.6	0.0%	0.0%	0.0%
3,5-xylidine	230-636-6	7235-40-7	7235407	3602	Reach_2232	882	5.14		1				-5.2	-5.0	-6.4	0.0%	0.0%	0.0%
benzylamine	246-376-1	24634-61-5	24634615	5792	Reach_2551	883	5.82	0.54	3	4.85	0.86		-5.2	-5.0	-6.1	0.0%	0.0%	0.0%
p-toluenesulphonyl isocyanate	223-810-8	4083-64-1	4083641	629	Reach_2011	884	5.11	0.75	4	4.11	0.75		-5.1	-5.0	-6.2	0.0%	0.0%	0.0%
cyclohex-1,4-ylenedimethanol	203-268-9	105-08-8	105088	1407	Reach_636	885	5.55		3	4.55			-4.4	-5.0	-6.6	0.0%	0.0%	0.0%
guaiacol	201-964-7	90-05-1	90051	3990	Reach_358	886	5.12	0.47	3	4.12	0.47		-5.2	-5.0	-6.6	0.0%	0.0%	0.0%
10,11-dihydro-5H-dibenz[b,f]azepine	601-145-8	111974-73-3	111974733	1566	Reach_4079	887	4.25		2				-4.6	-5.0	-6.6	0.0%	0.0%	0.0%
4-hydroxybenzoic acid	202-804-9	99-96-7	99967	1093	Reach_543	888	4.96	0.52	6	3.96	0.52		-4.4	-5.0	-6.6	0.0%	0.0%	0.0%
604-047-3	250-002-2	30018-16-7	30018167	5830	Reach_2641	889							-4.7	-5.0	-6.5	0.0%	0.0%	0.0%
geraniol	203-377-1	106-24-1	106241	186	Reach_661	890	4.30	0.23	5	3.44	0.69		-5.2	-5.0	-6.3	0.0%	0.0%	0.0%
glycerol trinitrate	200-240-8	55-63-0	55630	702	Reach_24	891	3.83	0.90	15	3.04	1.03	3	-5.2	-5.0	-6.7	0.0%	0.0%	0.0%
2-octyldodecan-1-ol	226-242-9	5333-42-6	5333426	3096	Reach_2098	892	4.09	1.73	3	1.76	1.24		-4.8	-5.0	-5.8	0.0%	0.0%	0.0%
dodec-1-ene	203-968-4	112-41-4	112414	1588	Reach_905	893	3.32	1.28	3	3.84	2.11		-5.3	-5.0	-7.3	0.0%	0.0%	0.0%
disodium 4,4'-bis[(4,6-dianilino-1,3,5-triazin-2-yl)amino]stilbene-	205-117-2	133-66-4	133664	5669	Reach_1124	894	5.63	0.25	3	4.63	0.25		-4.8	-5.0	-6.4	0.0%	0.0%	0.0%
2,9-dimethylanthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,1(	226-866-1	5521-31-3	5521313	3163	Reach_2121	895	5.13	2.03	3	4.13	2.03		-4.5	-5.0	-6.3	0.0%	0.0%	0.0%
hexahydro-2H-azepin-2-one, sodium salt	218-336-3	2123-24-2	2123242	5772	Reach_1759	896	6.18	0.42	3	5.18	0.42		-4.8	-5.0	-6.4	0.0%	0.0%	0.0%
trimethoxysilane	219-637-2	2487-90-3	2487903	563	Reach_1816	897	5.63	1.04	5	4.63	1.04		-5.3	-5.0	-6.3	0.0%	0.0%	0.0%
mercaptoacetic acid	200-677-4	68-11-1	68111	798	Reach_90	898	4.45	0.18	4	4.14	0.60		-4.1	-5.0	-6.7	0.0%	0.0%	0.0%
tetramethylammonium chloride	200-880-8	75-57-0	75570	1235	Reach_152	899	4.93	1.17	4	3.93	1.17		-4.8	-5.0	-6.4	0.0%	0.0%	0.0%
trichloroethylene	201-167-4	79-01-6	79016	909	Reach_223	900	4.77	0.48	32	4.03	0.86	6	-5.3	-5.0	-7.1	0.0%	0.0%	0.0%
isopropylamine	200-860-9	75-31-0	75310	855	Reach_138	901	5.24	0.63	6	3.62	0.70		-5.3	-5.0	-6.3	0.0%	0.0%	0.0%
2-naphthol	205-182-7	135-19-3	135193	435	Reach_1129	902	3.60	0.43	11	2.60	0.43	11	-5.2	-5.0	-6.6	0.0%	0.0%	0.0%
glycerol	200-289-5	56-81-5	56815	716	Reach_30	903	6.94	0.39	6	5.94	0.39		-4.3	-5.0	-6.7	0.0%	0.0%	0.0%
2,4-dihydro-5-methyl-2-phenyl-3H-pyrazol-3-imine	203-776-0	110-53-2	110532	1522	Reach_816	904	3.91		2				-5.0	-5.0	-6.5	0.0%	0.0%	0.0%
disodium 4,4'-diamino-9,9',10,10'-tetrahydro-9,9',10,10'-tetraox	227-877-4	6022-22-6	6022226	5946	Reach_2150	905							-4.8	-5.0	-6.4	0.0%	0.0%	0.0%
4-methoxybenzyl (6R,7R)-7-{[(2Z)-2-(5-amino-1,2,4-thiadiazol-3-\	700-025-3	102625-64-9	102625649	1348	Reach_4729	906	3.00	0.65	3				-4.7	-5.0	-6.5	0.0%	0.0%	0.0%
1-vinylimidazole	205-126-1	134-03-2	134032	5670	Reach_1126	907	4.87		1				-5.2	-5.0	-6.5	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
2-(2H-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)phenol	221-573-5	3147-75-9	3147759	2626	Reach_1920	908	4.19		1				-4.7	-5.0	-6.6	0.0%	0.0%	0.0%
benzenesulphonyl chloride	202-636-6	98-09-9	98099	1066	Reach_497	909	4.31	0.51	3	3.31	0.51		-5.2	-5.0	-6.4	0.0%	0.0%	0.0%
methanesulphonic acid	200-898-6	75-75-2	75752	3683	Reach_159	910	4.71	0.52	3	3.98	0.58		-4.2	-5.1	-6.6	0.0%	0.0%	0.0%
itaconic acid	202-599-6	97-65-4	97654	4168	Reach_484	911	4.96	0.73	3	3.96	0.73		-4.1	-5.1	-6.7	0.0%	0.0%	0.0%
1-chloro-1,1-difluoroethane	200-891-8	75-68-3	75683	3681	Reach_158	912	5.15	0.23	3	4.15	0.23		-5.5	-5.1	-7.3	0.0%	0.0%	0.0%
toluene-4-sulphonamide	200-741-1	70-55-3	70553	85	Reach_98	913	5.13	0.38	3	4.13	0.38		-4.8	-5.1	-6.1	0.0%	0.0%	0.0%
furan-2,5-dicarboxylic acid	221-800-8	3238-40-2	3238402	2650	Reach_1937	914	5.63	0.56	3				-4.2	-5.1	-6.7	0.0%	0.0%	0.0%
sodium 1,4-dicyclohexyl sulphonatosuccinate	245-629-3	23386-52-9	23386529	5785	Reach_2530	915	5.70		2				-4.8	-5.1	-6.4	0.0%	0.0%	0.0%
tetradecane	211-096-0	629-59-4	629594	3390	Reach_1468	916	5.93	2.47	3	4.93	2.47		-5.2	-5.1	-7.2	0.0%	0.0%	0.0%
(1S)-3-(dimethylamino)-1-(2-thienyl)propan-1-ol	608-570-8	31024-26-7	31024267	2616	Reach_4278	917	3.52	0.38	3				-4.3	-5.1	-6.8	0.0%	0.0%	0.0%
diisobutyl phthalate	201-553-2	84-69-5	84695	962	Reach_289	918	3.25	0.72	15	2.25	0.72		-5.3	-5.1	-6.3	0.0%	0.0%	0.0%
10-methoxy-5H-dibenz[b,f]azepine	202-447-9	95-75-0	95750	1038	Reach_440	919	3.73		2				-4.6	-5.1	-6.7	0.0%	0.0%	0.0%
613-175-9	700-035-8	6246-48-6	6246486	3371	Reach_4733	920	3.19	1.30	3				-4.8	-5.1	-6.6	0.0%	0.0%	0.0%
heptanoic acid	203-838-7	111-14-8	111148	293	Reach_845	921	5.24	0.63	3	4.24	0.63		-5.0	-5.1	-6.7	0.0%	0.0%	0.0%
decamethylenediamine	211-471-9	646-25-3	646253	3440	Reach_1484	922	3.95		2				-5.3	-5.1	-6.5	0.0%	0.0%	0.0%
611-084-9	211-519-9	657-27-2	657272	5975	Reach_1489	923							-4.5	-5.1	-6.6	0.0%	0.0%	0.0%
sodium 1-amino-4-bromo-9,10-dioxoanthracene-2-sulphonate	228-391-5	6258-06-6	6258066	5584	Reach_2158	924							-4.8	-5.1	-6.4	0.0%	0.0%	0.0%
4,4'-isopropylidenedicyclohexanol	201-244-2	80-04-6	80046	931	Reach_253	925	4.56	0.32	3	3.53	0.21		-4.8	-5.1	-6.0	0.0%	0.0%	0.0%
pyrene	204-927-3	129-00-0	129000	21	Reach_1114	926	1.95	1.19	6	0.95	0.70		-5.3	-5.1	-5.9	0.0%	0.0%	0.0%
N-phenylpiperazine	700-095-5	203448-76-4	203448764	2262	Reach_4759	927	4.07		1				-4.5	-5.1	-6.6	0.0%	0.0%	0.0%
bis(2-ethylhexyl) sebacate	204-558-8	122-62-3	122623	1755	Reach_1033	928	3.89	2.88	3	2.89	2.88		-5.1	-5.1	-5.7	0.0%	0.0%	0.0%
acetoacetanilide	202-996-4	102-01-2	102012	1334	Reach_587	929	5.34	0.24	3	4.41	0.72		-4.3	-5.1	-6.7	0.0%	0.0%	0.0%
bis(2-ethylhexyl) hydrogen phosphate	206-056-4	298-07-7	298077	592	Reach_1227	930	4.64	0.17	5	3.64	0.17		-5.0	-5.1	-6.0	0.0%	0.0%	0.0%
sodium butanolate	219-144-2	2372-45-4	2372454	5787	Reach_1787	931							-4.8	-5.1	-6.4	0.0%	0.0%	0.0%
potassium trifluoroacetate	220-877-5	2923-16-2	2923162	5822	Reach_1887	932	5.75	1.50	4	4.75	1.50		-4.8	-5.1	-6.4	0.0%	0.0%	0.0%
(Z)-octadec-9-enol	205-597-3	143-28-2	143282	1962	Reach_1192	933	4.48	2.00	3	3.48	2.00		-5.1	-5.1	-6.6	0.0%	0.0%	0.0%
potassium carbamoylcarbamate	247-728-7	26479-35-6	26479356	5805	Reach_2583	934	5.17	0.25	3	4.17	0.25		-4.8	-5.1	-6.4	0.0%	0.0%	0.0%
N-(2-bromo-4-fluorophenyl)acetamide	700-330-1	433733-92-7	433733927	2909	Reach_4864	935							-5.0	-5.1	-6.6	0.0%	0.0%	0.0%
zinc dilactate	240-178-9	16039-53-5	16039535	5730	Reach_2409	936	3.80	0.67	3	1.83	0.82		-4.8	-5.1	-6.4	0.0%	0.0%	0.0%
α,α,α,4-tetrachlorotoluene	210-258-8	611-19-8	611198	3326	Reach_1419	937	2.73	0.21	3	1.73	0.21		-5.3	-5.1	-6.7	0.0%	0.0%	0.0%
mequinol	205-769-8	150-76-5	150765	483	Reach_1204	938	4.49	0.84	24	3.49	0.84		-5.0	-5.1	-6.6	0.0%	0.0%	0.0%
5-amino-2,4,6-triiodoisophthalic acid	252-575-4	35453-19-1	35453191	2736	Reach_2691	939	3.92	0.39	3				-4.4	-5.1	-6.7	0.0%	0.0%	0.0%
N-(cyclohexylthio)phthalimide	241-774-1	17796-82-6	17796826	2153	Reach_2444	940	3.73	0.51	3	2.41	0.60		-4.4	-5.1	-6.6	0.0%	0.0%	0.0%
4-chloro-3-nitrobenzoic acid	603-565-7	132335-44-5	132335445	1857	Reach_4125	941	4.21	0.78	3				-4.5	-5.1	-6.8	0.0%	0.0%	0.0%
1,3-diphenyl-2-thiourea	203-004-2	102-08-9	102089	151	Reach_589	942	4.28	0.36	4	4.49	1.18		-5.0	-5.1	-5.9	0.0%	0.0%	0.0%
2,3,5-trimethylhydroquinone	206-441-7	342-25-6	342256	2695	Reach_1239	943	3.83	0.13	3	2.83	0.13		-5.0	-5.1	-6.6	0.0%	0.0%	0.0%
(2E,4R)-5-(biphenyl-4-yl)-4-[(tert-butoxycarbonyl)amino]-2-meth	605-866-9	179688-26-7	179688267	2160	Reach_4183	944	4.39	0.82	3				-4.7	-5.1	-6.5	0.0%	0.0%	0.0%
4,4'-[(isopropylidene)bis(p-phenyleneoxy)]diphthalic dianhydrid	253-781-7	38103-06-9	38103069	2816	Reach_2716	945	6.23		1				-4.8	-5.1	-5.6	0.0%	0.0%	0.0%
tris(2-ethylhexyl) phosphate	201-116-6	78-42-2	78422	895	Reach_199	946	4.34	0.69	4	3.34	0.69		-5.0	-5.1	-5.9	0.0%	0.0%	0.0%
17-hydroxypregna-4,9(11)-diene-3,20-dione	247-768-5	26537-19-9	26537199	2475	Reach_2586	947	3.43	0.58	3				-4.4	-5.1	-6.5	0.0%	0.0%	0.0%
bromoacetic acid	201-175-8	79-08-3	79083	912	Reach_228	948	3.89	1.13	5	3.85	0.94		-4.4	-5.1	-6.6	0.0%	0.0%	0.0%
1-(3-chlorophenyl)-4-(3-chloropropyl)piperazinium chloride	258-038-0	52605-52-4	52605524	5913	Reach_2785	949	5.38	0.93	3	4.38	0.93		-4.8	-5.1	-6.4	0.0%	0.0%	0.0%
iohexol	266-164-2	66108-95-0	66108950	80	Reach_2877	950	5.71	3.44	3				-4.3	-5.1	-6.4	0.0%	0.0%	0.0%
4-[[4-(aminocarbonyl)phenyl]azo]-N-(2-ethoxyphenyl)-3-hydroxy	220-509-3	2786-76-7	2786767	2520	Reach_1868	951	5.04	1.10	3	4.04	1.10		-4.9	-5.1	-6.7	0.0%	0.0%	0.0%
604-471-9	604-471-9	14543-49-8	14543498	1986	Reach_4155	952	4.40		2				-5.3	-5.1	-7.2	0.0%	0.0%	0.0%
citronellol	203-375-0	106-22-9	106229	185	Reach_659	953	3.93	0.48	3	3.39	0.60		-5.3	-5.1	-6.3	0.0%	0.0%	0.0%
2-(isopropylthio)-3-(2,2,2-trifluoroethoxy)pyridine	206-887-2	393-52-2	393522	2838	Reach_1264	954	4.21	0.89	3				-4.7	-5.1	-6.6	0.0%	0.0%	0.0%
3-hydroxy-N-(o-tolyl)-4-[(2,4,5-trichlorophenyl)azo]naphthalene-	229-440-3	6535-46-2	6535462	3451	Reach_2193	955	0.67	0.67	3				-5.1	-5.1	-5.6	0.0%	0.0%	0.0%
p-phenetidine	205-855-5	156-43-4	156434	2048	Reach_1213	956	3.84	0.65	3	2.84	0.65		-4.8	-5.1	-6.7	0.0%	0.0%	0.0%
cyclododeca-1,5,9-triene	225-533-8	4904-61-4	4904614	648	Reach_2067	957	3.69	0.77	5	2.69	0.77		-5.3	-5.1	-7.1	0.0%	0.0%	0.0%
2-[(p-aminophenyl)sulphonyl]ethyl hydrogensulphate	219-669-7	2494-89-5	2494895	2409	Reach_1820	958	5.18		1				-4.1	-5.1	-6.8	0.0%	0.0%	0.0%
potassium 1,2-bis(2-ethylhexyloxycarbonyl)ethanesulphonate	231-308-5	7491-09-0	7491090	6023	Reach_2256	959	4.58	0.23	3	3.58	0.23		-4.8	-5.1	-6.5	0.0%	0.0%	0.0%
naphthalene-1,8-dicarboxylic anhydride	201-380-2	81-84-5	81845	3816	Reach_280	960	5.58		1				-4.5	-5.1	-6.7	0.0%	0.0%	0.0%
620-313-1	221-738-1	3217-00-3	3217003	2643	Reach_1933	961							-4.6	-5.1	-6.6	0.0%	0.0%	0.0%
sodium dimethyl 5-sulphonatoisophthalate	223-578-8	3965-55-7	3965557	5872	Reach_2004	962	5.80	0.44	3	4.80	0.44		-4.8	-5.1	-6.5	0.0%	0.0%	0.0%
bis(dibutyldithiocarbamato-S,S')copper	237-695-7	13927-71-4	13927714	5685	Reach_2351	963							-4.8	-5.1	-6.5	0.0%	0.0%	0.0%
ethyl 2-cyano-2-phenyl-butanoate	611-342-0	55974-25-9	55974259	3183	Reach_4356	964	5.00		1				-5.3	-5.1	-6.6	0.0%	0.0%	0.0%
2,2-bis(allyloxymethyl)butan-1-ol	211-661-1	682-09-7	682097	3510	Reach_1499	965	5.74	0.38	3	4.75	0.42		-5.2	-5.1	-6.7	0.0%	0.0%	0.0%
603-923-2	603-923-2	135590-91-9	135590919	436	Reach_4133	966	3.88	0.41	5	2.84	0.44		-5.1	-5.1	-6.2	0.0%	0.0%	0.0%
600-024-7	231-501-4	7597-60-6	7597606	3691	Reach_2265	967							-4.8	-5.1	-6.5	0.0%	0.0%	0.0%
2,2,4,4-tetramethyl-7-oxa-3,20-diazadispiro[5.1.11.2]henicosan-	219-542-6	2458-08-4	2458084	1246	Reach_1813	968	5.37	0.22	3	4.37	0.22		-4.8	-5.1	-6.5	0.0%	0.0%	0.0%
N-methylformamide	204-624-6	123-39-7	123397	392	Reach_1048	969	6.85	0.70	8	5.85	0.70		-5.0	-5.1	-6.7	0.0%	0.0%	0.0%

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Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
610-954-5	200-261-2	56-18-8	56188	3188	Reach_25	970	5.26	0.54	3	4.33	0.35		-4.9	-5.1	-6.5	0.0%	0.0%	0.0%
amantadine hydrochloride	700-238-1	132900-75-5	132900755	1861	Reach_4815	971	1.60	0.82	3				-4.9	-5.1	-6.5	0.0%	0.0%	0.0%
calcium di(acetate)	259-393-4	54914-37-3	54914373	3156	Reach_2803	972	4.78	0.42	3	3.78	0.42		-4.9	-5.1	-6.5	0.0%	0.0%	0.0%
3-(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)propanal	204-092-5	115-46-8	115468	1637	Reach_942	973	5.17		1				-4.2	-5.1	-6.8	0.0%	0.0%	0.0%
p-menthane-1,8-diol	201-288-2	80-53-5	80535	3793	Reach_265	974	4.92	0.96	3				-4.5	-5.1	-6.7	0.0%	0.0%	0.0%
decyl oleate	222-981-6	3687-46-5	3687465	2782	Reach_1982	975	5.00		1				-5.3	-5.1	-5.5	0.0%	0.0%	0.0%
2-(methylamino)ethanol, compound with sulphur dioxide	244-311-1	21282-97-3	21282973	2288	Reach_2504	976	5.17	0.42	3	4.17	0.42		-4.9	-5.1	-6.5	0.0%	0.0%	0.0%
α,α,α-trichlorotoluene	210-275-0	611-70-1	611701	3328	Reach_1421	977	4.93	0.32	3	3.93	0.32		-5.3	-5.1	-6.6	0.0%	0.0%	0.0%
2,4,4-trimethylpentene	246-690-9	25167-70-8	25167708	2420	Reach_2561	978	3.03	0.21	3	2.03	0.21		-5.4	-5.1	-7.4	0.0%	0.0%	0.0%
chlorodimethylsilane	213-912-0	1066-35-9	1066359	1440	Reach_1637	979	5.50	0.25	3	4.51	0.26		-5.5	-5.1	-7.2	0.0%	0.0%	0.0%
2-morpholinoethanol	605-539-0	169115-74-6	169115746	5737	Reach_4178	980	5.33	0.30	3	4.33	0.30		-4.6	-5.1	-6.2	0.0%	0.0%	0.0%
tetradec-1-ene	214-306-9	1120-36-1	1120361	1569	Reach_1657	981	3.32	1.28	3	3.84	2.09		-5.3	-5.1	-7.2	0.0%	0.0%	0.0%
butane-1,3-diol	203-529-7	107-88-0	107880	1470	Reach_718	982	6.41	0.26	3	5.41	0.26		-4.6	-5.1	-6.7	0.0%	0.0%	0.0%
2,9-bis(3,5-dimethylphenyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoqu	225-590-9	4948-15-6	4948156	2983	Reach_2068	983	5.13	2.03	3	4.13	2.03		-5.0	-5.1	-6.4	0.0%	0.0%	0.0%
2,5-dimethylhexane-2,5-diol	203-731-5	110-03-2	110032	1513	Reach_802	984	6.83		1				-4.8	-5.1	-6.7	0.0%	0.0%	0.0%
1,2,4-trichlorobenzene	204-429-6	120-83-2	120832	363	Reach_1004	985	3.85	0.64	31	2.12	1.13	6	-5.4	-5.1	-6.7	0.0%	0.0%	0.0%
6-amino-1,3-dimethyluracil	202-046-9	91-17-8	91178	1005	Reach_371	986	3.35	0.70	16	2.67	0.70		-4.3	-5.1	-6.9	0.0%	0.0%	0.0%
strontium 3-hydroxy-4-[(4-methyl-2-sulphonatophenyl)azo]-2-na	277-552-6	73612-29-0	73612290	6016	Reach_2939	987	4.93	0.88	3	3.93	0.88		-4.9	-5.1	-6.5	0.0%	0.0%	0.0%
methyl stearate	203-990-4	112-61-8	112618	1595	Reach_916	988	0.99	0.73	3				-5.0	-5.1	-6.4	0.0%	0.0%	0.0%
7a-ethyldihydro-1H,3H,5H-oxazolo[3,4-c]oxazole	231-810-4	7747-35-5	7747355	880	Reach_2272	989	4.74	0.72	8	3.81	0.84		-5.1	-5.1	-6.5	0.0%	0.0%	0.0%
lactic acid	200-018-0	50-21-5	50215	654	Reach_4	990	5.56	0.46	6	4.56	0.46		-4.3	-5.1	-6.7	0.0%	0.0%	0.0%
1,2,3,6-tetrahydrophthalimide	201-602-8	85-40-5	85405	3888	Reach_293	991	5.94		1				-4.2	-5.1	-6.9	0.0%	0.0%	0.0%
3-((5-(3-(Dodecanoyloxy)-2,2-dimethylpropylideneamino)-1,3,3-t	700-071-4	932742-30-8	932742308	4067	Reach_4751	992	4.54	0.73	3	3.51	0.94		-5.3	-5.1	-3.2	0.0%	0.0%	0.1%
(+)-menthol	239-387-8	15356-60-2	15356602	486	Reach_2385	993	4.67	0.15	3	3.67	0.15		-5.3	-5.1	-6.5	0.0%	0.0%	0.0%
2-acrylamido-2-methylpropanesulphonic acid	239-268-0	15214-89-8	15214898	2021	Reach_2378	994	5.94	0.76	3	4.94	0.76		-4.1	-5.1	-6.7	0.0%	0.0%	0.0%
dilauroyl peroxide	203-326-3	105-74-8	105748	1419	Reach_648	995	-0.45	1.13	3				-5.2	-5.1	-5.9	0.0%	0.0%	0.0%
carbon tetrachloride	200-262-8	56-23-5	56235	710	Reach_26	996	4.47	0.85	15	4.44	0.66	6	-5.5	-5.1	-7.3	0.0%	0.0%	0.0%
2-propylvaleric acid	202-777-3	99-66-1	99661	1091	Reach_536	997	4.66	0.70	12	3.66	0.70		-5.0	-5.1	-6.8	0.0%	0.0%	0.0%
2-chloro-5-(trifluoromethyl)pyridine	257-856-5	52334-81-3	52334813	3058	Reach_2781	998	2.87	0.68	3				-4.6	-5.1	-6.7	0.0%	0.0%	0.0%
3-acetamido-5-amino-4-hydroxybenzenesulphonic acid	254-879-2	40306-75-0	40306750	2857	Reach_2730	999	5.39	0.26	3	4.39	0.26		-4.2	-5.1	-6.9	0.0%	0.0%	0.0%
2-nitro-4-(trifluoromethyl)benzonitrile	212-298-1	778-94-9	778949	3743	Reach_1545	1000	3.30	0.50	3	2.34	0.77		-5.3	-5.1	-6.7	0.0%	0.0%	0.0%
N,N-dibutylformamide	202-546-7	96-93-5	96935	4156	Reach_471	1001	5.86	0.65	3	4.86	0.65		-5.4	-5.1	-6.4	0.0%	0.0%	0.0%
2-sec-butylphenol	201-933-8	89-72-5	89725	993	Reach_350	1002	3.56	0.84	12	2.56	0.84		-5.4	-5.1	-6.1	0.0%	0.0%	0.0%
2'-methylacetoacetanilide	202-267-0	93-68-5	93685	4078	Reach_405	1003	5.52		2				-4.5	-5.1	-6.7	0.0%	0.0%	0.0%
617-448-3	230-437-4	7139-02-8	7139028	1288	Reach_2226	1004	3.73	0.07	3				-4.6	-5.1	-6.6	0.0%	0.0%	0.0%
2-chloro-3-methyl-4-(methylsulfonyl)benzoic acid	205-451-9	141-05-9	141059	454	Reach_1156	1005	4.61	0.36	4	3.61	0.36		-4.4	-5.1	-6.8	0.0%	0.0%	0.0%
600-451-9	205-844-5	155-41-9	155419	5717	Reach_1212	1006							-4.7	-5.1	-6.6	0.0%	0.0%	0.0%
docosanoic acid	204-010-8	112-85-6	112856	1608	Reach_927	1007	3.83	0.22	3	2.83	0.22		-5.2	-5.1	-6.2	0.0%	0.0%	0.0%
dipotassium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4-)	268-144-9	68015-77-0	68015770	5992	Reach_2896	1008	5.46	0.73	3	4.43	0.84		-4.9	-5.1	-6.5	0.0%	0.0%	0.0%
propylene carbonate	203-572-1	108-32-7	108327	1483	Reach_741	1009	4.59	1.08	3				-5.3	-5.1	-6.6	0.0%	0.0%	0.0%
bronopol	211-089-2	629-40-3	629403	771	Reach_1466	1010	5.53	0.33	3	4.53	0.33		-4.8	-5.1	-6.1	0.0%	0.0%	0.0%
4-(vinyloxy)butan-1-ol	241-793-5	17832-28-9	17832289	2154	Reach_2445	1011	4.69	0.21	3	3.81	0.21		-5.3	-5.1	-6.7	0.0%	0.0%	0.0%
diammonium dihydrogen ethylenediaminetetraacetate	244-063-4	20824-56-0	20824560	1204	Reach_2499	1012	5.27	0.81	4	4.58	1.03		-4.9	-5.1	-6.5	0.0%	0.0%	0.0%
dimethyl [3-[(hydroxymethyl)amino]-3-oxopropyl]phosphonate	243-528-9	20120-33-6	20120336	2250	Reach_2488	1013	5.97	0.73	3	4.97	0.73		-4.2	-5.1	-6.9	0.0%	0.0%	0.0%
barium 4-[(5-chloro-4-methyl-2-sulphonatophenyl)azo]-3-hydrox	231-494-8	7585-41-3	7585413	6029	Reach_2264	1014	5.28		1				-4.9	-5.1	-6.5	0.0%	0.0%	0.0%
triphenyl phosphite	202-908-4	101-02-0	101020	140	Reach_572	1015	2.75	0.27	5	1.75	0.27		-5.2	-5.1	-6.0	0.0%	0.0%	0.0%
sodium D-glycero-D-gulo-heptonate	235-849-8	13007-85-7	13007857	5656	Reach_2317	1016	6.08	0.73	3	5.08	0.73		-4.9	-5.1	-6.5	0.0%	0.0%	0.0%
trichloro(phenyl)silane	202-640-8	98-13-5	98135	1067	Reach_500	1017	6.13	0.90	3	4.16	0.51		-5.4	-5.1	-6.3	0.0%	0.0%	0.0%
vanillin	204-465-2	121-33-5	121335	369	Reach_1011	1018	4.93	0.21	4	3.93	0.21		-4.9	-5.2	-6.7	0.0%	0.0%	0.0%
1,5-naphthylene diisocyanate	221-641-4	3173-72-6	3173726	2631	Reach_1926	1019	4.44	1.45	3	3.44	1.45		-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
β,β-carotene	226-897-0	5537-71-3	5537713	3168	Reach_2123	1020	3.62	0.70	3				-5.4	-5.2	-3.6	0.0%	0.0%	0.0%
coumarin	202-086-7	91-64-5	91645	1008	Reach_377	1021	3.92	0.75	8	2.92	0.75		-5.3	-5.2	-6.7	0.0%	0.0%	0.0%
2-(morpholinothio)benzothiazole	244-017-3	20769-85-1	20769851	2273	Reach_2498	1022	4.65		2				-4.8	-5.2	-6.8	0.0%	0.0%	0.0%
dimethyl methylphosphonate	212-052-3	756-79-6	756796	3680	Reach_1526	1023	4.46	1.62	3				-5.3	-5.2	-6.6	0.0%	0.0%	0.0%
1-bromo-3-chloropropane	204-371-1	120-12-7	120127	358	Reach_989	1024	1.27	0.81	12	0.27	0.70	48	-5.4	-5.2	-6.7	0.0%	0.0%	0.0%
2,2'-[oxybis(methylene)]bis[2-ethylpropane-1,3-diol]	245-509-0	23235-61-2	23235612	2348	Reach_2529	1025	6.55		1				-4.3	-5.2	-6.8	0.0%	0.0%	0.0%
dipropylamine	205-565-9	142-84-7	142847	464	Reach_1181	1026	4.39	0.70	16	3.57	0.70		-5.4	-5.2	-6.2	0.0%	0.0%	0.0%
2-(4-tert-butylbenzyl)propionaldehyde	201-289-8	80-54-6	80546	3794	Reach_266	1027	3.86	0.49	3	2.96	0.36		-5.4	-5.2	-6.4	0.0%	0.0%	0.0%
N-(2-benzylphenyl)-2-chloroacetamide	239-784-6	15687-27-1	15687271	493	Reach_2393	1028	4.31	0.73	20	2.38	1.84	16	-4.6	-5.2	-6.8	0.0%	0.0%	0.0%
triisodecyl benzene-1,2,4-tricarboxylate	253-138-0	36631-30-8	36631308	2771	Reach_2701	1029	3.19		1	4.75			-5.4	-5.2	-4.8	0.0%	0.0%	0.0%
4-chloro-4'-hydroxybenzophenone	255-627-4	42019-78-3	42019783	2886	Reach_2748	1030	4.49	0.29	3	3.49	0.29		-5.1	-5.2	-6.4	0.0%	0.0%	0.0%
2-vinylpyridine	202-879-8	100-69-6	100696	1309	Reach_569	1031	4.29	0.32	3	3.16	0.77		-4.7	-5.2	-6.8	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
619-326-5	600-314-3	102445-69-2	102445692	1342	Reach_4059	1032	4.88	0.22	3				-4.2	-5.2	-7.0	0.0%	0.0%	0.0%
sodium p-[(4,6-dichloro-1,3,5-triazin-2-yl)amino]benzenesulphor	223-989-2	4156-21-2	4156212	5880	Reach_2017	1033	5.82	0.29	3	4.82	0.29		-4.9	-5.2	-6.5	0.0%	0.0%	0.0%
diethylamine	203-716-3	109-89-7	109897	5	Reach_796	1034	5.04	0.54	11	3.50	0.70	12	-5.4	-5.2	-6.2	0.0%	0.0%	0.0%
601-577-7	243-317-1	19794-93-5	19794935	2243	Reach_2485	1035	3.12	0.76	3				-4.9	-5.2	-6.5	0.0%	0.0%	0.0%
2-[(4-methoxy-2-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxobu	229-419-9	6528-34-3	6528343	3450	Reach_2192	1036	4.43	0.90	3	3.43	0.90		-4.5	-5.2	-6.6	0.0%	0.0%	0.0%
tetramethylenediamine	203-782-3	110-60-1	110601	1524	Reach_819	1037	4.81	0.68	3	3.81	0.68		-5.3	-5.2	-6.8	0.0%	0.0%	0.0%
dibenzyl ether	203-118-2	103-50-4	103504	1369	Reach_608	1038	3.44	0.50	3	2.44	0.50		-5.4	-5.2	-6.4	0.0%	0.0%	0.0%
sodium hydrogen N-(1-oxododecyl)-L-glutamate	249-958-3	29923-31-7	29923317	5828	Reach_2639	1039	5.16	0.60	3	4.16	0.60		-4.9	-5.2	-6.5	0.0%	0.0%	0.0%
3-chloroaniline	226-724-9	5459-04-1	5459041	1276	Reach_2114	1040	5.70		1				-5.0	-5.2	-6.0	0.0%	0.0%	0.0%
glutaral	203-856-5	111-30-8	111308	296	Reach_852	1041	3.72	0.65	12	3.71	0.27	4	-5.3	-5.2	-6.8	0.0%	0.0%	0.0%
valeric acid	203-677-2	109-52-4	109524	256	Reach_774	1042	4.82	0.35	5	3.82	0.35		-4.9	-5.2	-6.8	0.0%	0.0%	0.0%
2,2-bis[[(2-ethyl-1-oxohexyl)oxy]methyl]propane-1,3-diyl bis(2-e	230-743-8	7299-99-2	7299992	3611	Reach_2234	1043	0.09	1.56	3				-5.4	-5.2	-5.6	0.0%	0.0%	0.0%
2-decyltetradecanol	261-385-0	58670-89-6	58670896	3252	Reach_2831	1044	4.04	2.17	3	3.04	2.17		-5.3	-5.2	-5.6	0.0%	0.0%	0.0%
o-(trifluoromethyl)benzamide	206-637-2	360-64-5	360645	2756	Reach_1251	1045	3.86	0.94	3				-5.4	-5.2	-6.8	0.0%	0.0%	0.0%
pentan-3-one	202-490-3	96-22-0	96220	1048	Reach_455	1046	6.12	0.36	3	5.12	0.36		-5.4	-5.2	-6.3	0.0%	0.0%	0.0%
hexahydro-1,3,5-trimethyl-1,3,5-triazine	203-612-8	108-74-7	108747	1488	Reach_754	1047	3.72		2				-4.4	-5.2	-6.9	0.0%	0.0%	0.0%
685-281-3	685-281-3	2624-17-1	2624171	5804	Reach_4630	1048	6.52	0.45	3	5.52	0.45		-4.9	-5.2	-6.5	0.0%	0.0%	0.0%
didodecyl 3,3'-thiodipropionate	204-614-1	123-28-4	123284	1767	Reach_1043	1049	4.90	0.78	3	3.90	0.78		-5.4	-5.2	-5.6	0.0%	0.0%	0.0%
N-ethyl-p-methoxy-α-methylphenethylamine	611-084-9	54041-17-7	54041177	3118	Reach_4348	1050	3.47	1.74	3				-5.4	-5.2	-6.6	0.0%	0.0%	0.0%
dimethyl succinate	203-419-9	106-65-0	106650	1441	Reach_676	1051	5.45	0.34	3	4.40	0.15		-5.4	-5.2	-6.8	0.0%	0.0%	0.0%
tributyl citrate	201-071-2	77-94-1	77941	3745	Reach_191	1052	4.47	0.49	3	3.47	0.49		-4.7	-5.2	-6.7	0.0%	0.0%	0.0%
3-hydroxypropiononitrile	203-704-8	109-78-4	109784	1508	Reach_792	1053	5.29	1.10	3				-4.8	-5.2	-6.9	0.0%	0.0%	0.0%
α-methylcinnamaldehyde	202-938-8	101-39-3	101393	1320	Reach_576	1054	3.77	0.54	3	2.92	0.37		-5.4	-5.2	-6.4	0.0%	0.0%	0.0%
methyl acetoacetate	203-299-8	105-45-3	105453	1413	Reach_640	1055	5.39	0.71	3	4.39	0.71		-5.4	-5.2	-6.7	0.0%	0.0%	0.0%
dibutyl maleate	203-328-4	105-76-0	105760	183	Reach_650	1056	3.69	0.59	4	3.43	0.45		-5.4	-5.2	-6.6	0.0%	0.0%	0.0%
hexadecyl methacrylate	219-672-3	2495-27-4	2495274	2410	Reach_1821	1057	0.98	0.95	3	0.76			-5.1	-5.2	-6.4	0.0%	0.0%	0.0%
3,3'-[(2,5-dimethyl-p-phenylene)bis[imino(1-acetyl-2-oxoethylen	226-107-4	5280-80-8	5280808	3076	Reach_2092	1058	5.37	0.23	3	4.37	0.23		-5.6	-5.2	-6.2	0.0%	0.0%	0.0%
m-(4,5-dihydro-3-methyl-5-oxo-1H-pyrazol-1-yl)benzenesulphon	204-303-0	119-17-5	119175	1686	Reach_976	1059	5.35	0.61	3	4.35	0.61		-4.2	-5.2	-6.9	0.0%	0.0%	0.0%
1-propoxypropan-2-ol	216-372-4	1569-01-3	1569013	2052	Reach_1693	1060	6.48		1				-5.4	-5.2	-6.5	0.0%	0.0%	0.0%
(3R,4S,5R)-3,4,5-trihydroxycyclohex-1-enecarboxylic acid	700-265-9	2629-68-7	2629687	2463	Reach_4829	1061							-4.2	-5.2	-6.8	0.0%	0.0%	0.0%
4-chlorophenyl isocyanate	203-176-9	104-12-1	104121	1384	Reach_618	1062	3.59		2	2.96			-5.4	-5.2	-6.4	0.0%	0.0%	0.0%
605-539-0	210-734-5	622-40-2	622402	762	Reach_1445	1063	6.33	0.70	3	4.65	1.05		-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
5-sulphoanthranilic acid	601-161-5	112110-16-4	112110164	1574	Reach_4080	1064	4.25	0.76	3				-4.3	-5.2	-7.0	0.0%	0.0%	0.0%
3,5,6-tri-O-.benzyl-1,2-O-isopropylidene-α-D-glucofuranose	242-160-6	18282-59-2	18282592	2175	Reach_2456	1065	3.10		1				-4.7	-5.2	-6.4	0.0%	0.0%	0.0%
1,8-naphthylenediamine	207-529-8	479-27-6	479276	646	Reach_1291	1066	3.52	0.98	4	2.52	0.98		-5.0	-5.2	-6.0	0.0%	0.0%	0.0%
1,3-dichloropropan-2-ol	202-491-9	96-23-1	96231	1049	Reach_456	1067	5.73	0.33	3	4.73	0.33		-5.4	-5.2	-6.7	0.0%	0.0%	0.0%
sodium 1,2-diisobutoxycarbonylethanesulphonate	204-839-5	127-39-9	127399	5649	Reach_1097	1068	6.06		1				-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
ethyl 2-chloroacetoacetate	210-180-4	609-15-4	609154	3319	Reach_1415	1069	3.65		2				-5.4	-5.2	-6.6	0.0%	0.0%	0.0%
1,1'-(isopropylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)ben	244-617-5	21850-44-2	21850442	2307	Reach_2511	1070	0.66	2.87	3				-5.4	-5.2	-5.6	0.0%	0.0%	0.0%
Ethyl N-{[2-(chloromethyl)-1-methyl-1H-benzimidazol-5-yl]carbo	233-897-4	10420-33-4	10420334	1387	Reach_2292	1071	4.93	0.50	3	3.93	0.50		-4.7	-5.2	-6.8	0.0%	0.0%	0.0%
2-(11H-dibenzo[b,e]azepin-6-ylmethyl)-1H-isoindole-1,3(2H)-dio	218-056-1	2043-57-4	2043574	2264	Reach_1748	1072	2.77	0.32	3				-4.7	-5.2	-6.8	0.0%	0.0%	0.0%
616-309-4	204-516-9	122-03-2	122032	377	Reach_1025	1073	4.16	0.31	4	3.16	0.31		-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
morpholinium sulphamate	258-061-6	52636-67-6	52636676	5915	Reach_2786	1074	5.50		3	4.50			-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
N,N'''-1,6-hexanediylbis[N'-cyanoguanidine]	240-032-4	15894-70-9	15894709	2065	Reach_2404	1075	4.44	0.48	3	3.44	0.48		-4.3	-5.2	-6.7	0.0%	0.0%	0.0%
choline hydrogen carbonate	201-137-0	78-73-9	78739	6039	Reach_206	1076	5.70		1	4.73			-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
2,2'-dimorpholinyldiethyl ether	229-194-7	6425-39-4	6425394	3432	Reach_2184	1077	5.78	0.63	3	4.78	0.63		-4.3	-5.2	-7.0	0.0%	0.0%	0.0%
cyclohexyldimethylamine	202-715-5	98-94-2	98942	1080	Reach_525	1078	4.24	0.80	4	3.15	0.70		-5.5	-5.2	-6.5	0.0%	0.0%	0.0%
triethyl citrate	201-070-7	77-93-0	77930	92	Reach_190	1079	5.51	1.05	3	4.37	0.18		-5.0	-5.2	-6.8	0.0%	0.0%	0.0%
oxybispropanediol	261-605-5	59113-36-9	59113369	3265	Reach_2834	1080	6.16	1.64	3				-4.3	-5.2	-7.0	0.0%	0.0%	0.0%
5-ethylidene-8,9,10-trinorborn-2-ene	240-347-7	16219-75-3	16219753	2083	Reach_2414	1081	3.65	0.23	3	2.65	0.23		-5.5	-5.2	-7.2	0.0%	0.0%	0.0%
trioctyl benzene-1,2,4-tricarboxylate	201-877-4	89-04-3	89043	3967	Reach_337	1082	4.76	0.68	3	3.76	0.68		-5.4	-5.2	-5.6	0.0%	0.0%	0.0%
diethyl chloromalonate	229-014-7	6401-97-4	6401974	3422	Reach_2177	1083	1.71	2.81	3				-5.4	-5.2	-6.6	0.0%	0.0%	0.0%
tetrasodium hydrogen 2-phosphonatobutane-1,2,4-tricarboxylat	266-442-3	66669-53-2	66669532	5983	Reach_2883	1084	6.06	0.89	3	5.06	0.89		-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
methylphosphonic acid	213-607-2	993-13-5	993135	4203	Reach_1627	1085	4.99	0.99	3	4.60	1.02		-4.5	-5.2	-6.5	0.0%	0.0%	0.0%
2-ethylhexane-1,3-diol	234-129-0	10545-99-0	10545990	6391	Reach_2296	1086							-5.3	-5.2	-6.7	0.0%	0.0%	0.0%
p-(1,1-dimethylpropyl)phenol	201-280-9	80-46-6	80466	936	Reach_263	1087	3.42	0.84	24	2.38	0.84		-5.4	-5.2	-6.1	0.0%	0.0%	0.0%
dodecyldimethylamine	203-943-8	112-18-5	112185	321	Reach_892	1088	2.15	0.75	4	1.39	0.99		-5.5	-5.2	-7.3	0.0%	0.0%	0.0%
618-465-9	618-465-9	9011-11-4	9011114	5587	Reach_4495	1089							-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
cyclododecanone	212-595-6	830-13-7	830137	3840	Reach_1559	1090	3.80	0.24	3	2.77	0.59		-5.5	-5.2	-7.1	0.0%	0.0%	0.0%
bis(2-butoxyethyl) adipate	224-518-3	4394-85-8	4394858	2918	Reach_2031	1091	6.81	0.65	3	5.81	0.65		-5.4	-5.2	-6.7	0.0%	0.0%	0.0%
tetradecyl myristate	221-787-9	3234-85-3	3234853	2648	Reach_1936	1092	2.76	2.87	3	1.76	2.87		-5.4	-5.2	-5.6	0.0%	0.0%	0.0%
dimethyl 5-nitroisophthalate	616-149-5	74860-00-7	74860007	3648	Reach_4424	1093	5.00		1				-5.4	-5.2	-6.8	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
methyl undec-10-enoate	203-910-8	111-81-9	111819	1558	Reach_872	1094	3.09	0.49	3	2.09	0.49		-5.5	-5.2	-6.6	0.0%	0.0%	0.0%
tetrahydrothiophene	203-728-9	110-01-0	110010	271	Reach_800	1095	5.01	0.45	3	4.01	0.45		-5.5	-5.2	-6.5	0.0%	0.0%	0.0%
2,9-bis[4-(phenylazo)phenyl]anthra[2,1,9-def:6,5,10-d'e'f']diisoq	221-264-5	3049-71-6	3049716	2600	Reach_1907	1096	5.36	1.90	3	4.36	1.90		-5.6	-5.2	-6.5	0.0%	0.0%	0.0%
sodium [N-[2-[bis(carboxymethyl)amino]ethyl]-N-(2-hydroxyeth	257-036-7	51181-50-1	51181501	5903	Reach_2770	1097	5.06	0.69	3	4.94	0.43		-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
(6R-trans)-7-amino-3-methyl-8-oxo-5-thia-1-azabicyclo[4.2.0]oct	210-765-4	623-03-0	623030	763	Reach_1447	1098	4.68	0.34	4	3.68	0.34		-4.2	-5.2	-6.9	0.0%	0.0%	0.0%
3,5-dichloronitrobenzene	225-139-6	4684-28-0	4684280	2958	Reach_2055	1099	4.74	1.05	3				-5.5	-5.2	-6.2	0.0%	0.0%	0.0%
silver docosanoate	211-792-4	696-29-7	696297	809	Reach_1512	1100	3.47	0.07	3				-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
4-methylpentan-2-ol	203-551-7	108-11-2	108112	230	Reach_729	1101	5.61	0.34	5	4.59	0.41		-5.5	-5.2	-6.3	0.0%	0.0%	0.0%
aziridine	205-793-9	151-56-4	151564	485	Reach_1208	1102	3.97	0.57	4	2.95	0.68		-5.4	-5.2	-6.2	0.0%	0.0%	0.0%
2,4,6-triallyloxy-1,3,5-triazine	202-936-7	101-37-1	101371	1318	Reach_575	1103	4.11	0.29	3	3.31	0.20		-4.8	-5.2	-6.8	0.0%	0.0%	0.0%
D-N-(4-hydroxyphenyl)glycine	204-112-2	115-86-6	115866	9	Reach_946	1104	3.17	0.84	23	1.96	0.74	4	-4.2	-5.2	-6.9	0.0%	0.0%	0.0%
tetrasodium 7,7'-(carbonyldiimino)bis[4-hydroxy-3-[(6-sulphonat	249-171-5	28706-25-4	28706254	5817	Reach_2622	1105	5.20	0.83	3	4.20	0.83		-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
Methyl 5-methyl-4-[(oxomethylene)sulfamoyl]thiophene-3-carb	618-297-6	897671-34-0	897671340	3985	Reach_4491	1106	4.25	1.21	3				-4.6	-5.2	-6.8	0.0%	0.0%	0.0%
1,1,1-trichloroethane	200-756-3	71-55-6	71556	822	Reach_104	1107	4.99	0.61	18	4.03	1.05	7	-5.6	-5.2	-7.3	0.0%	0.0%	0.0%
3-hydroxy-2-naphthanilide	204-280-7	118-83-2	118832	1680	Reach_972	1108	3.52		1				-4.7	-5.2	-6.6	0.0%	0.0%	0.0%
7-hydroxynaphthalene-1-sulphonic acid	700-329-6	146763-69-1	146763691	1993	Reach_4863	1109	3.47	0.23	3				-4.3	-5.2	-7.0	0.0%	0.0%	0.0%
3-hydroxy-2-naphthoic acid	202-180-8	92-70-6	92706	4045	Reach_389	1110	4.74	0.25	3	3.79	0.40		-4.7	-5.2	-6.9	0.0%	0.0%	0.0%
isopropyl palmitate	205-571-1	142-91-6	142916	1957	Reach_1185	1111	5.91	1.93	3	4.91	1.93		-5.2	-5.2	-6.8	0.0%	0.0%	0.0%
oleic acid, compound with (Z)-N-octadec-9-enylpropane-1,3-dian	248-704-9	27871-49-4	27871494	2521	Reach_2613	1112	5.94	0.47	3	4.94	0.47		-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
3-methylbut-2-en-1-ol	209-141-4	556-82-1	556821	3176	Reach_1369	1113	5.32	0.47	3	4.32	0.47		-5.4	-5.2	-6.5	0.0%	0.0%	0.0%
3-Bromo-1-(3-chloropyridin-2-yl)-1H-pyrazole-5-carboxylic acid	481-150-8	500011-86-9	500011869	2992	Reach_4012	1114	4.74		1				-4.6	-5.2	-6.8	0.0%	0.0%	0.0%
sodium 4-(methoxycarbonyl)phenolate	225-714-1	5026-62-0	5026620	5897	Reach_2070	1115	4.73	0.28	3	3.73	0.28		-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
{5-chloro-2-[(cyclopropylmethyl)amino]phenyl}(phenyl)methanc	201-332-0	81-19-6	81196	939	Reach_273	1116	3.18	0.57	3	2.18	0.70		-4.9	-5.2	-6.1	0.0%	0.0%	0.0%
suberonitrile	700-912-5	895525-76-5	895525765	3979	Reach_5025	1117	2.65	0.47	3				-5.5	-5.2	-6.1	0.0%	0.0%	0.0%
2,4,8,10-tetra(tert-butyl)-6-hydroxy-12H-dibenzo[d,g][1,3,2]diox	286-344-4	85209-91-2	85209912	6058	Reach_2984	1118	4.36	0.40	3	3.53	0.53		-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
2-methyl-4-nitroimidazole	203-026-2	102-36-3	102363	1341	Reach_592	1119	3.98	1.19	3	3.75	0.82		-4.3	-5.2	-7.0	0.0%	0.0%	0.0%
benzyl salicylate	204-262-9	118-58-1	118581	1674	Reach_966	1120	3.14	0.24	3	2.35	0.13		-5.2	-5.2	-6.7	0.0%	0.0%	0.0%
tris[(2-hydroxyethyl)ammonium] citrate	244-599-9	21829-50-5	21829505	5774	Reach_2509	1121	4.83	1.19	3	3.91	1.57		-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
O-acetylsalicylic acid	200-064-1	50-78-2	50782	666	Reach_9	1122	5.25	0.48	7	3.25	0.57		-4.6	-5.2	-6.8	0.0%	0.0%	0.0%
4-hydroxy-5-[[(p-tolyl)sulphonyl]amino]naphthalene-2,7-disulph	200-085-6	51-21-8	51218	668	Reach_13	1123	3.24	3.23	5	2.24	3.23		-4.3	-5.2	-7.0	0.0%	0.0%	0.0%
4-[(2,5-dichlorophenyl)azo]-3-hydroxy-N-phenylnaphthalene-2-c	227-930-1	6041-94-7	6041947	3310	Reach_2151	1124	5.07	1.38	3	4.07	1.38		-5.2	-5.2	-5.7	0.0%	0.0%	0.0%
calcium 4,5-dichloro-2-[[4,5-dihydro-3-methyl-5-oxo-1-(3-sulpho	213-234-5	931-36-2	931362	4059	Reach_1607	1125	5.09	0.30	3	4.20	0.46		-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
sodium diisobutyldithiophosphinate	236-419-2	13360-78-6	13360786	5667	Reach_2331	1126	5.18	0.40	3	4.18	0.40		-5.0	-5.2	-6.6	0.0%	0.0%	0.0%
pentafluoroethane	206-557-8	354-33-6	354336	2733	Reach_1246	1127	5.60	0.26	3	4.12	0.51		-5.6	-5.3	-7.5	0.0%	0.0%	0.0%
2,2'-azobis[2-methylpropionamidine] dihydrochloride	221-070-0	2997-92-4	2997924	5829	Reach_1895	1128	4.08	1.13	3	3.08	1.13		-5.0	-5.3	-6.6	0.0%	0.0%	0.0%
zinc diricinoleate	235-911-4	13040-19-2	13040192	5659	Reach_2319	1129	2.79	0.84	4	1.79	0.84		-5.0	-5.3	-6.6	0.0%	0.0%	0.0%
[[4-[[4-(anilino)phenyl][4-(phenylimino)-2,5-cyclohexadien-1-ylid	215-385-2	1324-76-1	1324761	1858	Reach_1677	1130	0.88	0.52	3				-4.9	-5.3	-6.8	0.0%	0.0%	0.0%
N,N-dimethylaniline	261-619-1	59130-69-7	59130697	3268	Reach_2835	1131	0.87	0.41	3				-5.4	-5.3	-6.1	0.0%	0.0%	0.0%
maleic acid	203-742-5	110-16-7	110167	275	Reach_806	1132	4.83	0.64	6	3.83	0.75		-4.3	-5.3	-6.9	0.0%	0.0%	0.0%
p-(dimethoxymethyl)anisole	218-577-4	2186-92-7	2186927	2308	Reach_1770	1133	5.22	0.28	3	4.38	0.36		-5.4	-5.3	-6.7	0.0%	0.0%	0.0%
bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate	258-207-9	52829-07-9	52829079	3077	Reach_2788	1134	3.69	0.43	3	2.81	0.86		-4.9	-5.3	-6.4	0.0%	0.0%	0.0%
1-chloro-2,5-dimethoxybenzene	218-267-9	2100-42-7	2100427	2282	Reach_1758	1135	4.11		2				-5.5	-5.3	-6.4	0.0%	0.0%	0.0%
6-methoxy-m-toluidine	204-419-1	120-71-8	120718	1718	Reach_1000	1136	4.53		1				-4.7	-5.3	-6.8	0.0%	0.0%	0.0%
1,1,3,3-tetramethylbutylamine	203-491-1	107-45-9	107459	220	Reach_708	1137	4.19	0.22	4	3.19	0.22		-5.5	-5.3	-7.5	0.0%	0.0%	0.0%
benzyl acetate	205-399-7	140-11-4	140114	448	Reach_1147	1138	4.13	0.63	4	3.13	0.63		-5.5	-5.3	-6.5	0.0%	0.0%	0.0%
!4-methylmorpholine 4-oxide! !monohydrate!	231-391-8	7529-22-8	7529228	3663	Reach_2258	1139	7.49		1	3.97			-4.3	-5.3	-7.0	0.0%	0.0%	0.0%
6,6',6''-(1,3,5-triazine-2,4,6-triyltriimino)trihexanoic acid	279-505-5	80584-91-4	80584914	3795	Reach_2959	1140	6.09		1				-4.8	-5.3	-6.8	0.0%	0.0%	0.0%
bis(piperidinothiocarbonyl) hexasulphide	213-537-2	971-15-3	971153	4161	Reach_1621	1141	1.74	1.80	3				-4.9	-5.3	-6.7	0.0%	0.0%	0.0%
(1S,3R,7S,8S,8aR)-8-{2-[(2R,4R)-4-hydroxy-6-oxotetrahydro-2H-p	220-374-0	2743-38-6	2743386	2506	Reach_1862	1142	4.48	0.85	3				-4.7	-5.3	-6.5	0.0%	0.0%	0.0%
617-251-2	250-439-9	31027-31-3	31027313	2618	Reach_2651	1143	3.94	0.76	3	3.61	1.01		-4.4	-5.3	-7.0	0.0%	0.0%	0.0%
isoquinoline	204-341-8	119-65-3	119653	356	Reach_984	1144	4.27	0.24	6	3.27	0.24		-5.1	-5.3	-6.8	0.0%	0.0%	0.0%
2,2,6,6-tetramethyl-4-piperidylamine	202-678-5	98-53-3	98533	4186	Reach_510	1145	4.22	0.44	3	3.22	0.44		-5.5	-5.3	-6.8	0.0%	0.0%	0.0%
3-chloropropyl(dimethyl)amine	239-349-0	15307-93-4	15307934	2029	Reach_2383	1146	2.87		2				-5.5	-5.3	-6.4	0.0%	0.0%	0.0%
(Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine	203-749-3	110-25-8	110258	1515	Reach_809	1147	3.47	0.63	3	2.56	0.70		-4.7	-5.3	-6.8	0.0%	0.0%	0.0%
2-ethyl-2-[[(1-oxoallyl)oxy]methyl]-1,3-propanediyl diacrylate	239-701-3	15625-89-5	15625895	2046	Reach_2391	1148	3.71	0.54	3	2.71	0.54		-5.5	-5.3	-6.8	0.0%	0.0%	0.0%
di(succinimido) carbonate	604-349-5	143382-03-0	143382030	1964	Reach_4149	1149							-4.4	-5.3	-7.0	0.0%	0.0%	0.0%
1,3-diphenylguanidine	203-002-1	102-06-7	102067	1335	Reach_588	1150	3.98	0.49	3	2.74	0.91		-4.9	-5.3	-6.8	0.0%	0.0%	0.0%
605-014-6	605-014-6	1555-62-0	1555620	2042	Reach_4166	1151	4.17		1				-4.8	-5.3	-6.9	0.0%	0.0%	0.0%
2-imidazolidone	200-074-6	50-98-6	50986	5902	Reach_11	1152	5.12	0.48	3	4.12	0.48		-5.2	-5.3	-6.8	0.0%	0.0%	0.0%
dimethyl 2-nitroterephthalate	226-134-1	5292-45-5	5292455	680	Reach_2094	1153	3.73	0.72	6	2.73	0.72		-5.5	-5.3	-6.9	0.0%	0.0%	0.0%
betaine	203-490-6	107-43-7	107437	1462	Reach_707	1154	6.39		2				-4.2	-5.3	-7.0	0.0%	0.0%	0.0%
3,4-diaminobenzenesulphonic acid	239-138-3	15086-94-9	15086949	2013	Reach_2376	1155	2.15	1.08	3				-4.4	-5.3	-7.0	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
2,4,6-tris(dimethylaminomethyl)phenol	202-013-9	90-72-2	90722	4003	Reach_366	1156	5.37	0.43	3	4.37	0.43		-4.5	-5.3	-6.9	0.0%	0.0%	0.0%
pin-2(3)-ene	201-291-9	80-56-8	80568	937	Reach_267	1157	3.94	1.14	5	2.94	1.14		-5.5	-5.3	-7.4	0.0%	0.0%	0.0%
disodium 2-hydroxyethyliminodi(acetate)	617-500-5	83905-01-5	83905015	957	Reach_4465	1158	2.40	2.49	5	1.40	1.29		-5.0	-5.3	-6.6	0.0%	0.0%	0.0%
l-Glutamic acid, N-coco acyl derivs., monosodium salts	269-087-2	68187-32-6	68187326	5994	Reach_2900	1159	5.40	0.62	3	4.40	0.62		-5.0	-5.3	-6.6	0.0%	0.0%	0.0%
2-nitropropane	201-209-1	79-46-9	79469	921	Reach_247	1160	5.45	0.61	4	4.77	0.85		-5.5	-5.3	-6.4	0.0%	0.0%	0.0%
[7(S)-(1α,.2β,4β,5α,7β)]-3-oxa-9-azatricyclo[3.3.1.02,4]non-7-yl (	241-475-6	17462-58-7	17462587	2140	Reach_2433	1161	4.31	0.44	3				-4.4	-5.3	-7.0	0.0%	0.0%	0.0%
4-chlorotoluene	202-809-6	100-00-5	100005	119	Reach_546	1162	3.93	0.70	32	2.91	0.86		-5.5	-5.3	-7.1	0.0%	0.0%	0.0%
ethylenediamine-N,N'-bis((2-hydroxyphenyl)acetic acid)	225-195-1	4708-04-7	4708047	1271	Reach_2057	1163	5.03	0.58	3				-4.3	-5.3	-7.0	0.0%	0.0%	0.0%
calcium diethyl bis[[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl	260-353-3	56718-70-8	56718708	3210	Reach_2820	1164	4.57	0.26	3				-5.0	-5.3	-6.6	0.0%	0.0%	0.0%
607-145-4	607-578-9	25157-64-6	25157646	2418	Reach_4244	1165	2.87	3.61	3				-5.5	-5.3	-6.4	0.0%	0.0%	0.0%
618-837-0	618-837-0	92339-11-2	92339112	6408	Reach_4501	1166							-5.0	-5.3	-6.7	0.0%	0.0%	0.0%
triphenylphosphine oxide	614-050-1	67330-25-0	67330250	3489	Reach_4394	1167	2.76	0.26	3				-5.2	-5.3	-6.1	0.0%	0.0%	0.0%
2,6-dimethyloct-7-en-2-ol	242-362-4	18479-58-8	18479588	2192	Reach_2463	1168	4.64	0.19	3	3.70	0.39		-5.5	-5.3	-6.5	0.0%	0.0%	0.0%
dapsone	201-248-4	80-08-0	80080	3787	Reach_256	1169	4.00	0.81	3	3.00	0.81		-4.5	-5.3	-6.9	0.0%	0.0%	0.0%
5-(methoxymethyl)pyridine-2,3-dicarboxylic acid	203-801-5	110-76-9	110769	1530	Reach_827	1170	5.25		2				-4.5	-5.3	-7.0	0.0%	0.0%	0.0%
3-Bromo-5-chlorophenol	206-337-1	328-84-7	328847	2665	Reach_1235	1171	3.28		2				-5.5	-5.3	-6.9	0.0%	0.0%	0.0%
8,9,10,11-tetrachloro-12H-phthaloperin-12-one	244-007-9	20749-68-2	20749682	2272	Reach_2497	1172	6.17	1.10	3	5.17	1.10		-5.1	-5.3	-6.1	0.0%	0.0%	0.0%
3-amino-5-chloro-2-hydroxybenzenesulphonic acid	228-169-8	6153-06-6	6153066	1280	Reach_2155	1173	3.56	1.09	3				-4.3	-5.3	-7.0	0.0%	0.0%	0.0%
butyric acid	203-532-3	107-92-6	107926	224	Reach_719	1174	5.44	0.63	5	4.44	0.56		-5.0	-5.3	-6.9	0.0%	0.0%	0.0%
O,O-diethyl phosphorochloridothioate	246-309-6	24549-06-2	24549062	2397	Reach_2549	1175	4.49	0.28	3	3.49	0.28		-5.5	-5.3	-6.5	0.0%	0.0%	0.0%
3-chloro-o-toluidine	252-276-9	34893-92-0	34893920	2717	Reach_2684	1176	3.65	0.45	3	2.65	0.45		-4.8	-5.3	-6.9	0.0%	0.0%	0.0%
2,2',6,6'-tetrabromo-4,4'-isopropylidenediphenol	201-236-9	79-94-7	79947	929	Reach_252	1177	2.57	0.56	7	2.41	0.73		-4.6	-5.3	-5.6	0.0%	0.0%	0.0%
3,5-dinitrobenzoic acid	700-313-9	21134-38-3	21134383	2283	Reach_4855	1178							-4.5	-5.3	-7.0	0.0%	0.0%	0.0%
hyoscine	605-999-2	18361-03-0	18361030	2185	Reach_4188	1179	5.16	0.35	3				-4.4	-5.3	-7.0	0.0%	0.0%	0.0%
2-butyl-2-ethylpropanediol	204-111-7	115-84-4	115844	1639	Reach_945	1180	4.97		1				-4.9	-5.3	-6.8	0.0%	0.0%	0.0%
5,5-dimethylhydantoin	201-051-3	77-71-4	77714	883	Reach_181	1181	6.37	1.12	3	5.37	1.12		-4.7	-5.3	-6.7	0.0%	0.0%	0.0%
chlorhexidine	200-238-7	55-56-1	55561	3175	Reach_23	1182	2.11	0.81	3	1.26	1.02		-4.8	-5.3	-6.5	0.0%	0.0%	0.0%
6,6'-di-tert-butyl-2,2'-methylenedi-p-cresol	204-327-1	119-47-1	119471	1692	Reach_978	1183	1.70	1.14	3				-4.9	-5.3	-6.0	0.0%	0.0%	0.0%
methylpentynol	201-055-5	77-75-8	77758	885	Reach_183	1184	5.85	0.74	12	4.85	0.74	12	-5.5	-5.3	-6.2	0.0%	0.0%	0.0%
3-(dimethylamino)-1-(thiophen-2-yl)propan-1-ol	207-185-9	447-61-0	447610	2932	Reach_1277	1185	3.67	0.37	3				-4.5	-5.3	-7.0	0.0%	0.0%	0.0%
bis(2-dimethylaminoethyl)(methyl)amine	221-201-1	3030-47-5	3030475	2590	Reach_1898	1186	4.98	0.26	3	4.21	0.21		-5.5	-5.3	-7.0	0.0%	0.0%	0.0%
sodium 3-[(1,5-dihydroxy-2-naphthyl)azo]-4-hydroxybenzenesul	229-114-0	6413-10-1	6413101	1284	Reach_2180	1187	4.82	1.08	3				-5.0	-5.3	-6.7	0.0%	0.0%	0.0%
tamoxifen	234-118-0	10540-29-1	10540291	174	Reach_2294	1188	1.76	0.13	3				-5.1	-5.3	-6.0	0.0%	0.0%	0.0%
3,3',5,5'-tetramethylbiphenyl-2,2'-diol	628-771-4	23357-46-2	23357462	2349	Reach_4589	1189	4.25		1				-4.9	-5.3	-6.6	0.0%	0.0%	0.0%
N,N'-di-sec-butyl-p-phenylenediamine	202-992-2	101-96-2	101962	1331	Reach_585	1190	2.76	0.39	3	1.74	0.35		-5.5	-5.3	-6.5	0.0%	0.0%	0.0%
3,5-dimethylpyrazole	200-657-5	67-51-6	67516	3494	Reach_82	1191	5.50		3	4.50			-4.5	-5.3	-6.8	0.0%	0.0%	0.0%
bis(2-ethylhexyl) maleate	205-524-5	142-16-5	142165	1948	Reach_1172	1192	4.47	1.18	3	3.47	1.18		-5.3	-5.3	-7.0	0.0%	0.0%	0.0%
sulisobenzone	235-469-2	12237-63-7	12237637	5628	Reach_2309	1193	3.08	1.54	3	2.08	1.54		-4.6	-5.3	-6.4	0.0%	0.0%	0.0%
Methyl dec-9-enoate	231-658-9	7680-73-1	7680731	6032	Reach_2268	1194							-5.5	-5.3	-6.7	0.0%	0.0%	0.0%
Benzyl [(3aS,4R,6S,6aR)-6-hydroxy-2,2-dimethyltetrahydro-3aH-	700-224-5	1647-12-7	1647127	2093	Reach_4810	1195	3.91	0.65	3				-4.7	-5.3	-6.8	0.0%	0.0%	0.0%
1-(3-sulphonatopropyl)pyridinium	239-491-3	15471-17-7	15471177	2039	Reach_2389	1196	7.62	1.20	3	6.62	1.20		-4.5	-5.3	-6.9	0.0%	0.0%	0.0%
butan-2-one O,O',O''-(methylsilylidyne)trioxime	245-366-4	22984-54-9	22984549	2341	Reach_2525	1197	5.11	0.76	3	3.94	0.83		-5.3	-5.3	-5.8	0.0%	0.0%	0.0%
3-methyl-2-butenal	203-527-6	107-86-8	107868	1469	Reach_716	1198	4.19	0.14	3	3.43	0.16		-5.5	-5.3	-6.6	0.0%	0.0%	0.0%
methacrylamide	201-202-3	79-39-0	79390	3775	Reach_244	1199	6.44		1				-4.9	-5.3	-7.0	0.0%	0.0%	0.0%
bis(2-(2-methoxyethoxy)ethyl) ether	205-594-7	143-24-8	143248	28	Reach_1191	1200	7.00	0.36	3	6.00	0.36		-4.9	-5.3	-7.0	0.0%	0.0%	0.0%
TCA (reach)	211-479-2	650-51-1	650511	1230	Reach_1486	1201	5.93	1.02	11	5.68	2.75	3	-5.1	-5.3	-6.7	0.0%	0.0%	0.0%
fenofibrate	618-126-5	88196-70-7	88196707	3950	Reach_4487	1202	4.72		1				-5.4	-5.3	-6.3	0.0%	0.0%	0.0%
627-082-6	627-082-6	89878-14-8	89878148	3989	Reach_4583	1203							-5.6	-5.3	-6.6	0.0%	0.0%	0.0%
benzoxonium chloride	243-008-1	19379-90-9	19379909	5758	Reach_2478	1204							-5.1	-5.3	-6.7	0.0%	0.0%	0.0%
isopropyl oleate	203-935-4	112-11-8	112118	1575	Reach_888	1205	5.00		1	5.00			-5.2	-5.3	-6.4	0.0%	0.0%	0.0%
2-(bromomethyl)-2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxolane	262-103-9	60207-89-8	60207898	3308	Reach_2846	1206	2.94	0.52	3				-5.4	-5.3	-6.6	0.0%	0.0%	0.0%
3-(trimethoxysilyl)propyl isocyanate	239-415-9	15396-00-6	15396006	2033	Reach_2387	1207	5.12	0.90	3	4.12	0.90		-5.2	-5.3	-7.0	0.0%	0.0%	0.0%
Ethyl 3-amino-4-[2-(phthalimido)ethoxy]crotonate	238-339-3	14367-46-5	14367465	1969	Reach_2364	1208	3.56	0.66	3				-4.4	-5.3	-7.0	0.0%	0.0%	0.0%
salbutamol	242-424-0	18559-94-9	18559949	2198	Reach_2465	1209	3.40	0.96	3				-4.4	-5.3	-7.0	0.0%	0.0%	0.0%
605-637-3	222-818-9	3621-82-7	3621827	2762	Reach_1976	1210	2.74		1				-4.5	-5.3	-7.0	0.0%	0.0%	0.0%
601-262-4	601-262-4	1135-22-4	1135224	1622	Reach_4082	1211							-4.6	-5.3	-7.0	0.0%	0.0%	0.0%
paracetamol	281-339-3	83929-47-9	83929479	3853	Reach_2968	1212	3.07	0.50	3				-4.8	-5.3	-6.1	0.0%	0.0%	0.0%
4-(3-methyl-5-oxo-2-pyrazolin-1-yl)benzenesulphonic acid	203-607-0	108-69-0	108690	244	Reach_753	1213	4.10	0.42	4	3.10	0.42		-4.3	-5.3	-7.0	0.0%	0.0%	0.0%
4-morpholinecarbaldehyde	205-466-0	141-18-4	141184	1934	Reach_1159	1214	3.80	0.36	3	2.80	0.36		-4.3	-5.3	-7.0	0.0%	0.0%	0.0%
[hexane-1,6-diylbis[nitrilobis(methylene)]]tetrakisphosphonic ac	254-135-7	38820-59-6	38820596	5871	Reach_2718	1215	5.75		2	5.12			-5.1	-5.3	-6.7	0.0%	0.0%	0.0%
1,3-dihydro-5-methoxy-2H-benzimidazole-2-thione	253-326-2	37052-78-1	37052781	2789	Reach_2709	1216	4.49	0.76	3	3.49	0.76		-4.6	-5.3	-7.0	0.0%	0.0%	0.0%
604-848-8	700-822-6	1026785-65-8	1026785658	1350	Reach_5001	1217	2.71	0.31	3				-4.8	-5.3	-7.0	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
618-706-8	202-445-8	95-73-8	95738	4131	Reach_438	1218	4.13		2	3.30			-5.3	-5.3	-6.7	0.0%	0.0%	0.0%
4-hydroxynaphthalene-1-sulphonic acid	680-587-3	144163-97-3	144163973	1972	Reach_4626	1219	4.24	0.80	3				-4.3	-5.3	-7.0	0.0%	0.0%	0.0%
6-hydroxynaphthalene-2-sulphonic acid	646-413-5	144689-24-7	144689247	1977	Reach_4613	1220	3.18	0.99	3				-4.3	-5.3	-7.0	0.0%	0.0%	0.0%
N-(4-chloro-2,5-dimethoxyphenyl)-3-hydroxy-4-[[2-methoxy-5-[(	226-103-2	5280-68-2	5280682	3074	Reach_2090	1221	5.04	1.10	3	4.04	1.10		-5.0	-5.3	-6.9	0.0%	0.0%	0.0%
1,2,3,6-tetrahydro-4-methylphthalic anhydride	222-323-8	3425-89-6	3425896	2699	Reach_1960	1222	5.01		2				-5.5	-5.3	-6.9	0.0%	0.0%	0.0%
(Z)-pent-2-enenitrile	229-353-0	6485-55-8	6485558	3445	Reach_2190	1223	5.27	0.21	3	4.34	0.45		-5.6	-5.3	-6.5	0.0%	0.0%	0.0%
2-mercaptoethanol	200-464-6	60-24-2	60242	749	Reach_56	1224	4.22	1.12	4	3.22	1.12		-5.5	-5.3	-6.9	0.0%	0.0%	0.0%
bis(4-(1,1,3,3-tetramethylbutyl)phenyl)amine	239-816-9	15721-78-5	15721785	2055	Reach_2395	1225	4.45	0.39	3	3.45	0.39		-4.5	-5.3	-6.8	0.0%	0.0%	0.0%
heptanal	203-898-4	111-71-7	111717	1554	Reach_867	1226	3.89	0.62	3	2.89	0.62		-5.6	-5.3	-6.7	0.0%	0.0%	0.0%
6-methyl-1,3,5-triazine-2,4-diyldiamine	267-135-7	67801-15-4	67801154	3500	Reach_2889	1227	3.63	0.50	3	2.79	0.53		-4.6	-5.3	-6.6	0.0%	0.0%	0.0%
4-(methylsulfonyl)-2-nitrobenzoic acid	601-017-1	110964-79-9	110964799	1534	Reach_4077	1228	5.71	0.41	3	4.71	0.41		-4.4	-5.3	-7.1	0.0%	0.0%	0.0%
2-[2-(Piperazin-1-yl)ethoxy]ethanol	224-970-1	4584-46-7	4584467	5891	Reach_2049	1229							-4.5	-5.3	-7.0	0.0%	0.0%	0.0%
azacyclonol	608-748-5	324763-46-4	324763464	2653	Reach_4281	1230	2.70	1.02	3				-4.7	-5.3	-6.8	0.0%	0.0%	0.0%
ethyltriphenylfosfonium bromide	214-447-6	1129-42-6	1129426	1612	Reach_1663	1231	5.70		1				-5.6	-5.3	-6.6	0.0%	0.0%	0.0%
pivaloyl chloride	221-921-6	3282-30-2	3282302	601	Reach_1941	1232	4.90	1.22	3	3.90	0.75		-5.6	-5.3	-7.0	0.0%	0.0%	0.0%
N-(2,5-dimethoxyphenyl)acetamide	203-955-3	112-29-8	112298	324	Reach_895	1233	3.57	1.24	3	2.57	1.24		-4.6	-5.3	-7.0	0.0%	0.0%	0.0%
ethyl (S)-2-hydroxypropionate	211-694-1	687-47-8	687478	3526	Reach_1503	1234	5.96	0.41	3	5.00	0.17		-5.5	-5.3	-6.8	0.0%	0.0%	0.0%
2,9-dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione	221-424-4	3089-17-6	3089176	2615	Reach_1916	1235	5.18	0.72	3	4.18	0.72		-5.1	-5.3	-6.6	0.0%	0.0%	0.0%
benzoin	204-331-3	119-53-9	119539	1694	Reach_979	1236	4.32	0.22	3	3.32	0.22		-4.6	-5.3	-6.9	0.0%	0.0%	0.0%
pentane-2,4-dione	204-634-0	123-54-6	123546	395	Reach_1052	1237	4.99	0.26	17	3.25	0.63	6	-5.5	-5.3	-6.9	0.0%	0.0%	0.0%
anthranilic acid	204-287-5	118-92-3	118923	1683	Reach_974	1238	4.92	0.59	3	3.92	0.59		-4.6	-5.3	-7.0	0.0%	0.0%	0.0%
4-amino-2,5-dimethoxy-N-methylbenzenesulphonamide	256-435-3	49701-24-8	49701248	2986	Reach_2763	1239	3.86	1.71	3				-4.4	-5.3	-7.0	0.0%	0.0%	0.0%
dimethyl(tetradecyl)amine	204-002-4	112-75-4	112754	1601	Reach_922	1240	1.99	0.89	3	1.16	0.86		-5.5	-5.3	-7.6	0.0%	0.0%	0.0%
trimethyl orthoformate	205-745-7	149-73-5	149735	480	Reach_1201	1241	5.73	0.75	4	5.34	0.75		-5.6	-5.3	-6.6	0.0%	0.0%	0.0%
4,4'-oxydi(benzenesulphonohydrazide)	201-286-1	80-51-3	80513	3792	Reach_264	1242	3.62	0.82	3	2.37	0.23		-4.4	-5.3	-7.1	0.0%	0.0%	0.0%
methanesulphonyl chloride	204-706-1	124-63-0	124630	404	Reach_1079	1243	4.27	0.23	5	3.27	0.23		-5.6	-5.3	-6.6	0.0%	0.0%	0.0%
isobutyl acetate	203-745-1	110-19-0	110190	277	Reach_808	1244	5.32	0.49	4	4.28	0.75		-5.6	-5.3	-6.7	0.0%	0.0%	0.0%
cyclopentanone	204-435-9	120-92-3	120923	364	Reach_1005	1245	6.59	0.60	3	5.59	0.60		-5.5	-5.3	-6.4	0.0%	0.0%	0.0%
2-[(1R,4R,4aS,8aR)-4,7-dimethyl-1,2,3,4,4a,5,6,8a-octahydronapl	609-904-5	41263-74-5	41263745	2874	Reach_4315	1246	4.95	0.70	3				-4.8	-5.3	-6.9	0.0%	0.0%	0.0%
2-hydroxy-2-methylpropiophenone	231-272-0	7473-98-5	7473985	3642	Reach_2253	1247	4.61	1.39	3	3.61	1.39		-5.1	-5.3	-7.0	0.0%	0.0%	0.0%
cyclododecane	206-033-9	294-62-2	294622	587	Reach_1225	1248	4.33	0.70	12	1.96	0.70		-5.5	-5.3	-7.4	0.0%	0.0%	0.0%
4-amino-2,5-dimethoxy-N-phenylbenzenesulphonamide	257-821-4	52298-44-9	52298449	3056	Reach_2779	1249	6.70		1				-4.6	-5.3	-7.0	0.0%	0.0%	0.0%
2-(propyloxy)ethanol	220-548-6	2807-30-9	2807309	2522	Reach_1870	1250	5.61	0.86	3				-5.5	-5.3	-6.9	0.0%	0.0%	0.0%
1,3-dioxolane	211-463-5	646-06-0	646060	780	Reach_1482	1251	7.00		1	5.74			-5.6	-5.3	-6.8	0.0%	0.0%	0.0%
decane	204-686-4	124-18-5	124185	402	Reach_1072	1252	4.95	2.36	7	3.95	0.70		-5.6	-5.3	-7.7	0.0%	0.0%	0.0%
N-(trimethylsilyl)imidazole	610-491-9	500011-92-7	500011927	2993	Reach_4330	1253	3.51	1.36	3				-5.6	-5.3	-6.6	0.0%	0.0%	0.0%
p-benzoquinone	203-405-2	106-51-4	106514	197	Reach_673	1254	2.07	0.48	3	1.07	0.68		-5.5	-5.3	-7.0	0.0%	0.0%	0.0%
phthalic acid	224-427-9	4355-11-7	4355117	1268	Reach_2029	1255	4.39	0.24	3				-4.7	-5.4	-6.9	0.0%	0.0%	0.0%
616-206-4	600-709-0	106006-84-2	106006842	1424	Reach_4071	1256	4.00	0.60	3				-4.9	-5.4	-7.0	0.0%	0.0%	0.0%
perylene-3,4:9,10-tetracarboxylic dianhydride	204-905-3	128-69-8	128698	1822	Reach_1112	1257	5.13	2.03	3	4.13	2.03		-5.0	-5.4	-6.5	0.0%	0.0%	0.0%
1-(1-methyl-2-propoxyethoxy)propan-2-ol	249-949-4	29911-27-1	29911271	2577	Reach_2636	1258	5.12	0.57	3				-5.6	-5.4	-6.8	0.0%	0.0%	0.0%
2,2'-iminobis[4,6-diamino-1,3,5-triazine]	222-695-1	3576-88-3	3576883	2746	Reach_1973	1259	4.54	0.11	3	3.54	0.11		-4.6	-5.4	-6.7	0.0%	0.0%	0.0%
{5-chloro-2-[(cyclopropylmethyl)amino]phenyl}(phenyl)methanc	618-944-2	93413-69-5	93413695	1019	Reach_4503	1260	3.32	0.79	3	2.32	0.79		-5.3	-5.4	-6.4	0.0%	0.0%	0.0%
610-029-6	206-564-6	354-58-5	354585	2737	Reach_1248	1261	4.10	0.10	3				-4.4	-5.4	-7.1	0.0%	0.0%	0.0%
2-(octylthio)ethanol	222-598-4	3547-33-9	3547339	613	Reach_1970	1262	3.10	0.41	5	1.87	0.50		-5.5	-5.4	-6.5	0.0%	0.0%	0.0%
N-[4-(aminocarbonyl)phenyl]-4-methoxy-3-nitrobenzamide	298-790-7	93839-20-4	93839204	4087	Reach_2999	1263							-4.5	-5.4	-7.0	0.0%	0.0%	0.0%
potassium O-isobutyl dithiocarbonate	676-405-7	165253-31-6	165253316	2097	Reach_4616	1264	4.65	0.97	3				-5.1	-5.4	-6.7	0.0%	0.0%	0.0%
2,6-dichlorobenzoxazole	210-557-3	618-62-2	618622	759	Reach_1438	1265	3.36	0.70	16	2.36	0.70		-5.6	-5.4	-6.4	0.0%	0.0%	0.0%
4-aminobenzoic acid	205-753-0	150-13-0	150130	2007	Reach_1203	1266	4.08	0.80	3				-4.6	-5.4	-7.0	0.0%	0.0%	0.0%
undecan-4-olide	203-225-4	104-67-6	104676	1398	Reach_626	1267	4.17	0.44	3	3.35	0.60		-5.6	-5.4	-6.5	0.0%	0.0%	0.0%
2-ethylhexyl cyanoacetate	236-425-5	13361-34-7	13361347	1870	Reach_2332	1268	4.09	0.40	3	3.27	0.73		-5.6	-5.4	-6.7	0.0%	0.0%	0.0%
butylamine	203-699-2	109-73-9	109739	263	Reach_787	1269	4.73	0.88	9	3.42	0.70		-5.6	-5.4	-6.4	0.0%	0.0%	0.0%
S-allyl 5-amino-4-(2-methylphenyl)-3-oxo-2,3-dihydro-1H-pyrazo	203-472-8	107-20-0	107200	215	Reach_699	1270	3.59	0.70	7	2.59	0.70		-4.5	-5.4	-7.0	0.0%	0.0%	0.0%
N-(1,1-dimethyl-3-oxobutyl)acrylamide	220-713-2	2873-97-4	2873974	2542	Reach_1879	1271	6.29		1				-4.5	-5.4	-7.0	0.0%	0.0%	0.0%
4,4'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[2,4-dihydr	222-530-3	3520-72-7	3520727	2725	Reach_1969	1272	1.48	1.81	3	3.00			-4.8	-5.4	-6.7	0.0%	0.0%	0.0%
3,5-diacetamido-2,4,6-triiodobenzoic acid	202-815-9	100-06-1	100061	1291	Reach_549	1273	4.92	0.24	3				-4.6	-5.4	-7.0	0.0%	0.0%	0.0%
[2-[[2-cyano-3-[4-(diethylamino)phenyl]-1-oxoallyl]oxy]ethyl][3-[	278-859-8	78181-99-4	78181994	6036	Reach_2953	1274	4.25	0.42	3	3.23	0.55		-5.1	-5.4	-6.7	0.0%	0.0%	0.0%
1,3-diethyl-2-thiourea	203-308-5	105-55-5	105555	178	Reach_642	1275	5.36	0.42	4	4.28	1.04		-5.0	-5.4	-6.2	0.0%	0.0%	0.0%
cyclohexanediacetic acid	203-892-1	111-65-9	111659	306	Reach_863	1276	2.35	0.84	4	1.35	0.70		-4.8	-5.4	-7.0	0.0%	0.0%	0.0%
2-({2-[(3-aminobenzoyl)amino]ethyl}sulfonyl)ethyl hydrogen sul	220-040-4	2612-57-9	2612579	2455	Reach_1847	1277	4.06	0.92	3	3.06	0.92		-4.4	-5.4	-7.0	0.0%	0.0%	0.0%
(3S-cis)-3,6-dimethyl-1,4-dioxane-2,5-dione	213-243-4	931-87-3	931873	4064	Reach_1609	1278	3.79	0.88	3	2.79	0.88		-4.6	-5.4	-6.9	0.0%	0.0%	0.0%
erythromycin thiocyanate	231-723-1	7704-67-8	7704678	1236	Reach_2271	1279	5.32		1	2.29			-5.1	-5.4	-6.7	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
cyclopentane	206-016-6	287-92-3	287923	2545	Reach_1222	1280	4.02	0.55	3	3.02	0.55		-5.6	-5.4	-7.7	0.0%	0.0%	0.0%
1-vinylhexahydro-2H-azepin-2-one	218-787-6	2235-00-9	2235009	2331	Reach_1777	1281	5.26	0.45	3	4.26	0.45		-5.5	-5.4	-6.9	0.0%	0.0%	0.0%
2,5-bis(p-toluidino)terephthalic acid	233-651-6	10291-28-8	10291288	1355	Reach_2287	1282	2.41	0.68	3				-4.9	-5.4	-7.0	0.0%	0.0%	0.0%
crotonaldehyde	224-030-0	4170-30-3	4170303	634	Reach_2018	1283	4.01	0.96	7	1.97	0.86		-5.6	-5.4	-6.7	0.0%	0.0%	0.0%
2-chlorotoluene	202-424-3	95-49-8	95498	1030	Reach_430	1284	4.19	0.61	9	3.19	0.84		-5.6	-5.4	-7.3	0.0%	0.0%	0.0%
ethyl cyanoacetate	203-309-0	105-56-6	105566	1415	Reach_643	1285	5.17	0.40	3	4.17	0.40		-5.5	-5.4	-6.9	0.0%	0.0%	0.0%
4-[(5-{[(benzyloxy)carbonyl]amino}pentyl)(hydroxy)amino]-4-oxo	600-744-1	106410-46-2	106410462	1435	Reach_4073	1286	4.30	0.89	3				-4.6	-5.4	-7.0	0.0%	0.0%	0.0%
methyl hydrogen 2-nitroterephthalate	252-360-5	35092-89-8	35092898	2722	Reach_2686	1287	4.46	0.94	3				-4.7	-5.4	-7.0	0.0%	0.0%	0.0%
2,5-dimethoxyaniline	256-380-5	49564-57-0	49564570	2984	Reach_2762	1288	5.49		1				-4.6	-5.4	-7.0	0.0%	0.0%	0.0%
1,2,4-trimethylbenzene	202-436-9	95-63-6	95636	1035	Reach_436	1289	3.68	0.70	24	2.68	0.70		-5.6	-5.4	-7.1	0.0%	0.0%	0.0%
7-methylenepentadecane	603-419-2	13043-55-5	13043555	1836	Reach_4119	1290	1.05	0.41	3				-5.3	-5.4	-7.1	0.0%	0.0%	0.0%
N,N,N',N'-tetramethyl-2,2'-oxybis(ethylamine)	221-220-5	3033-62-3	3033623	2592	Reach_1900	1291	4.67	0.79	3	3.67	0.79		-5.6	-5.4	-7.0	0.0%	0.0%	0.0%
disodium 4,5-dichloro-2-[[4,5-dihydro-3-methyl-5-oxo-1-(3-sulph	209-067-2	554-68-7	554687	5931	Reach_1363	1292							-5.1	-5.4	-6.7	0.0%	0.0%	0.0%
5-{5-chloro-3-[4-(methylsulfonyl)phenyl]pyridin-2-yl}-2-methylpy	202-225-1	93-17-4	93174	4063	Reach_400	1293	5.25	0.19	3	4.25	0.19		-5.1	-5.4	-6.7	0.0%	0.0%	0.0%
N-acetylsulphanilyl chloride	208-494-1	530-78-9	530789	3086	Reach_1327	1294	3.77		1				-4.7	-5.4	-7.0	0.0%	0.0%	0.0%
2-amino-2-methylpropanol	204-709-8	124-68-5	124685	1792	Reach_1081	1295	5.42	0.22	3	4.42	0.22		-5.4	-5.4	-7.0	0.0%	0.0%	0.0%
tetrapropylammonium bromide	217-727-6	1941-30-6	1941306	5759	Reach_1736	1296	5.44		1				-5.1	-5.4	-6.7	0.0%	0.0%	0.0%
allyl (2S,4S)-4-(benzoylthio)-2-(dimethylcarbamoyl)pyrrolidine-1-	204-255-0	118-48-9	118489	1671	Reach_964	1297	4.70	0.35	3	3.84	0.43		-4.7	-5.4	-7.0	0.0%	0.0%	0.0%
9-ethylcarbazole	671-709-6	430-67-1	430671	2905	Reach_4615	1298	4.14	0.70	3				-5.6	-5.4	-6.9	0.0%	0.0%	0.0%
6-(hydroxymethyl)-4-phenyl-3,4-dihydro-2H-chromen-2-ol	242-687-1	18936-17-9	18936179	2216	Reach_2472	1299	4.83	0.73	3				-4.6	-5.4	-7.0	0.0%	0.0%	0.0%
benzenesulphonamide	202-637-1	98-10-2	98102	4178	Reach_498	1300	4.55	1.38	3				-4.9	-5.4	-6.9	0.0%	0.0%	0.0%
1,2-dibromoethane	203-444-5	106-93-4	106934	202	Reach_683	1301	4.28	0.59	7	3.28	0.70		-5.6	-5.4	-7.0	0.0%	0.0%	0.0%
(2-hydroxyethyl)ammonium mercaptoacetate	204-815-4	126-97-6	126976	5647	Reach_1092	1302	5.07	0.74	3	4.07	0.74		-5.1	-5.4	-6.7	0.0%	0.0%	0.0%
triethylammonium chloride	619-636-0	125971-57-5	125971575	1800	Reach_4534	1303	3.43	0.31	3	2.13	0.46		-5.1	-5.4	-6.7	0.0%	0.0%	0.0%
2-(benzylmethylamino)ethyl acetoacetate	207-151-3	445-03-4	445034	2926	Reach_1276	1304	3.85		1				-5.3	-5.4	-7.1	0.0%	0.0%	0.0%
benzyl butyl phthalate	201-622-7	85-68-7	85687	968	Reach_299	1305	2.95	0.51	18	2.17	0.47	4	-5.5	-5.4	-6.7	0.0%	0.0%	0.0%
dibutyl phthalate	201-557-4	84-74-2	84742	963	Reach_290	1306	3.17	0.50	26	2.43	0.30	7	-5.6	-5.4	-6.8	0.0%	0.0%	0.0%
sodium 2-butyloctyl sulphate	303-553-9	94200-74-5	94200745	6090	Reach_3008	1307	4.19	0.65	3	3.19	0.65		-5.1	-5.4	-6.7	0.0%	0.0%	0.0%
601-145-8	230-961-3	7384-80-7	7384807	3628	Reach_2245	1308	2.74	2.02	3				-5.1	-5.4	-6.7	0.0%	0.0%	0.0%
1,4-dimethoxybenzene	205-771-9	150-78-7	150787	484	Reach_1205	1309	4.84	0.70	20	3.84	0.70		-5.6	-5.4	-6.7	0.0%	0.0%	0.0%
(1S)-1,2,3,4-tetrahydronaphthalen-1-amine	201-258-9	80-20-6	80206	3789	Reach_260	1310	3.75	0.49	3				-5.6	-5.4	-6.6	0.0%	0.0%	0.0%
(1R)-1,2,3,4-tetrahydronaphthalen-1-amine	617-178-6	80841-78-7	80841787	3799	Reach_4447	1311	3.77	1.35	3				-5.6	-5.4	-6.6	0.0%	0.0%	0.0%
D-glucono-1,5-lactone	202-016-5	90-80-2	90802	4006	Reach_367	1312	5.68	0.28	3	4.68	0.28		-4.5	-5.4	-7.2	0.0%	0.0%	0.0%
propylphosphonic acid	225-121-8	4672-38-2	4672382	2957	Reach_2054	1313	5.17	0.27	3	4.17	0.27		-4.6	-5.4	-7.0	0.0%	0.0%	0.0%
dimethyl sebacate	203-431-4	106-79-6	106796	1446	Reach_678	1314	3.75	0.34	3	2.85	0.51		-5.6	-5.4	-6.5	0.0%	0.0%	0.0%
1,3-dichlorobenzene	208-792-1	541-73-1	541731	685	Reach_1341	1315	4.25	0.54	16	3.22	0.48	6	-5.6	-5.4	-7.1	0.0%	0.0%	0.0%
methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	228-985-4	6386-38-5	6386385	3420	Reach_2176	1316	3.82	0.56	3	2.82	0.56		-5.4	-5.4	-6.7	0.0%	0.0%	0.0%
2,6-dichloro-N-phenylaniline	203-787-0	110-64-5	110645	1527	Reach_823	1317	5.30	0.43	3	4.30	0.43		-5.6	-5.4	-6.8	0.0%	0.0%	0.0%
diethyl ether--boron trifluoride	201-265-7	80-26-2	80262	934	Reach_261	1318	4.39	0.48	3	3.39	0.48		-5.1	-5.4	-6.7	0.0%	0.0%	0.0%
succinic anhydride	203-570-0	108-30-5	108305	1481	Reach_739	1319	5.29	0.34	3	4.29	0.34		-5.2	-5.4	-7.0	0.0%	0.0%	0.0%
sodium 3-mercaptopropanesulphonate	241-620-3	17636-10-1	17636101	5741	Reach_2438	1320	7.98		1	7.88			-5.1	-5.4	-6.7	0.0%	0.0%	0.0%
619-799-8	614-977-1	69477-29-8	69477298	6002	Reach_4404	1321							-5.6	-5.4	-6.7	0.0%	0.0%	0.0%
calcium bis[4-[[1-[[(2-chlorophenyl)amino]carbonyl]-2-oxopropyl	276-057-2	71832-85-4	71832854	6011	Reach_2932	1322	3.69	1.39	3	2.69	1.39		-5.1	-5.4	-6.8	0.0%	0.0%	0.0%
methyl myristate	210-412-4	615-16-7	615167	3336	Reach_1425	1323	5.17		1				-5.6	-5.4	-7.0	0.0%	0.0%	0.0%
difluoromethane	200-839-4	75-10-5	75105	3657	Reach_130	1324	5.96	0.43	3	3.87	0.46		-5.9	-5.4	-7.5	0.0%	0.0%	0.0%
6,10-dimethylundeca-3,5,9-trien-2-one	205-457-1	141-10-6	141106	1932	Reach_1157	1325	3.53	0.29	3	2.79	0.34		-5.6	-5.4	-6.7	0.0%	0.0%	0.0%
pentane-1,5-diol	203-854-4	111-29-5	111295	1545	Reach_851	1326	6.67		1				-4.8	-5.4	-7.0	0.0%	0.0%	0.0%
601-329-8	247-832-2	26591-72-0	26591720	5806	Reach_2590	1327	5.89	1.66	3	4.89	1.66		-4.9	-5.4	-6.7	0.0%	0.0%	0.0%
2-phenylethanol	200-456-2	60-12-8	60128	3306	Reach_55	1328	5.63	0.28	3	4.82	0.27		-5.6	-5.4	-6.9	0.0%	0.0%	0.0%
2-chlorophenyl isocyanate	612-101-2	61203-94-9	61203949	3329	Reach_4371	1329	2.58	0.13	3				-5.6	-5.4	-6.7	0.0%	0.0%	0.0%
α-[2-(methylamino)ethyl]benzyl alcohol	207-223-4	454-31-9	454319	2940	Reach_1278	1330	3.84		1				-4.9	-5.4	-7.1	0.0%	0.0%	0.0%
methyl (3R,5S,6E)-7-{4-(4-fluorophenyl)-6-isopropyl-2-[methyl(m	201-757-1	87-61-6	87616	979	Reach_313	1331	3.36	0.70	36	2.27	0.49		-4.8	-5.4	-7.0	0.0%	0.0%	0.0%
2,6-difluoro-3-[(propylsulfonyl)amino]benzoic acid	700-740-0	1103234-56-5	1103234565	1517	Reach_4982	1332	3.86	0.89	3				-4.7	-5.4	-7.1	0.0%	0.0%	0.0%
2,4-dichloro-5-sulphamoylbenzoic acid	600-906-1	109232-37-3	109232373	1497	Reach_4076	1333	3.39	0.54	3				-4.6	-5.4	-7.1	0.0%	0.0%	0.0%
methyl 5-nitrohydrogen.isophthalate	217-793-6	1955-46-0	1955460	2235	Reach_1739	1334	5.24	0.79	3	4.24	0.79		-4.7	-5.4	-7.1	0.0%	0.0%	0.0%
3-amino-4-chlorobenzoic acid	695-654-2	1012341-48-8	1012341488	1316	Reach_4692	1335	4.08		2				-4.7	-5.4	-7.1	0.0%	0.0%	0.0%
2-chloro-N-(2,6-dichlorophenyl)-N-phenylacetamide	223-460-6	3905-19-9	3905199	2832	Reach_2000	1336	-1.98	4.24	3	4.00			-5.5	-5.4	-6.7	0.0%	0.0%	0.0%
1,1,1,3,3,3-hexamethyldisilazane	213-668-5	999-97-3	999973	1096	Reach_1631	1337	5.11	0.90	3	4.19	0.75		-5.9	-5.4	-7.6	0.0%	0.0%	0.0%
5-Chloro-1,3-dimethyl-1H-pyrazole-4-carbonyl chloride	203-907-1	111-78-4	111784	311	Reach_871	1338	3.86	0.55	5	2.93	0.60		-4.7	-5.4	-7.1	0.0%	0.0%	0.0%
hexyl salicylate	228-408-6	6259-76-3	6259763	3375	Reach_2159	1339	2.80	0.26	3	2.01	0.27		-5.5	-5.4	-6.8	0.0%	0.0%	0.0%
octadecyl acrylate	225-383-3	4813-57-4	4813574	2971	Reach_2064	1340	5.15	0.26	3	4.56	0.15		-5.3	-5.4	-6.6	0.0%	0.0%	0.0%
2-amino-4-chlorophenol	604-434-7	144689-93-0	144689930	1978	Reach_4152	1341	4.23	1.21	3				-4.7	-5.4	-7.1	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
619-779-9	607-657-8	252317-48-9	252317489	5796	Reach_4246	1342							-4.7	-5.4	-7.1	0.0%	0.0%	0.0%
methyl palmitate	203-966-3	112-39-0	112390	1586	Reach_903	1343	5.74		1				-5.5	-5.4	-7.0	0.0%	0.0%	0.0%
icos-1-ene	249-220-0	28783-41-7	28783417	5818	Reach_2624	1344	5.00		1				-5.5	-5.4	-6.4	0.0%	0.0%	0.0%
4-aminoazobenzene	600-261-6	101990-44-7	101990447	1333	Reach_4058	1345	3.20	1.05	3				-5.3	-5.4	-6.3	0.0%	0.0%	0.0%
4-amino-5-hydroxynaphthalene-2,7-disulphonic acid	800-428-5	1256387-74-2	1256387742	1798	Reach_5045	1346	3.33	0.10	3				-4.4	-5.4	-7.0	0.0%	0.0%	0.0%
2-amino-5-chlorophenol	604-568-6	147118-40-9	147118409	1995	Reach_4157	1347	3.40	0.57	3				-4.7	-5.4	-7.1	0.0%	0.0%	0.0%
608-385-2	600-141-3	1009-22-9	1009229	1311	Reach_4056	1348	3.59	0.83	3				-4.6	-5.4	-7.0	0.0%	0.0%	0.0%
(Z)-4-hydroxy-4-(6-methoxynaphthalen-2-yl)but-3-en-2-one	604-848-8	152402-98-7	152402987	2023	Reach_4164	1349	3.70	0.24	3	2.70	0.24		-4.6	-5.4	-7.0	0.0%	0.0%	0.0%
methyl carbamate	619-293-7	97845-60-8	97845608	4173	Reach_4512	1350	4.15	0.93	3				-5.5	-5.4	-7.0	0.0%	0.0%	0.0%
climbazole	253-775-4	38083-17-9	38083179	620	Reach_2715	1351	2.88	0.88	9	2.08	0.69		-5.2	-5.4	-6.3	0.0%	0.0%	0.0%
tetrapropylammonium hydroxide	224-800-6	4499-86-9	4499869	5889	Reach_2042	1352							-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
2-bromopropionic acid	202-063-1	91-35-0	91350	4015	Reach_375	1353	3.95	0.52	3				-4.5	-5.4	-7.1	0.0%	0.0%	0.0%
4-hydroxy-2,2,6,6-tetramethylpiperidine-1-ethanol	258-132-1	52722-86-8	52722868	3072	Reach_2787	1354	5.17	0.50	3	4.17	0.50		-4.7	-5.4	-7.0	0.0%	0.0%	0.0%
N,N-bis(2-hydroxyethyl)dodecanamide	204-393-1	120-40-1	120401	13	Reach_993	1355	3.61	0.37	3	2.59	0.36		-5.0	-5.4	-6.9	0.0%	0.0%	0.0%
Ethyl 2-amino-4,5-bis(2-methoxyethoxy)benzoate	700-551-3	179688-27-8	179688278	2161	Reach_4931	1356	4.76	0.51	3				-4.8	-5.4	-7.1	0.0%	0.0%	0.0%
lithium dodecyl sulphate	218-058-2	2044-56-6	2044566	5768	Reach_1749	1357	4.19	0.65	3	3.19	0.65		-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
propyl acetate	203-686-1	109-60-4	109604	258	Reach_779	1358	5.21	0.44	5	4.21	0.44		-5.6	-5.4	-6.8	0.0%	0.0%	0.0%
dodecyl methacrylate	205-570-6	142-90-5	142905	465	Reach_1184	1359	3.53	2.44	3	2.53	2.44		-5.6	-5.4	-7.2	0.0%	0.0%	0.0%
bis(2,4-dichloro-5-nitrophenyl) carbonate	254-471-4	39489-75-3	39489753	2841	Reach_2725	1360	2.03	0.89	3				-5.0	-5.4	-6.7	0.0%	0.0%	0.0%
diethyl oxalate	202-464-1	95-92-1	95921	1042	Reach_447	1361	4.27	1.21	4	2.82	0.70		-5.6	-5.4	-6.7	0.0%	0.0%	0.0%
isopropyl acetate	203-561-1	108-21-4	108214	233	Reach_734	1362	5.85	0.60	4	4.98	0.80		-5.6	-5.4	-6.9	0.0%	0.0%	0.0%
2,2'-dithiodi(benzoic acid)	246-563-8	25013-16-5	25013165	1208	Reach_2558	1363	3.50	0.84	32	2.50	0.84		-5.2	-5.4	-6.4	0.0%	0.0%	0.0%
2,3-epoxypropyl neodecanoate	247-979-2	26761-45-5	26761455	2487	Reach_2593	1364	3.63	0.30	3	2.63	0.30		-5.6	-5.4	-6.8	0.0%	0.0%	0.0%
4-Nitrophenyl 1,3-thiazol-5-ylmethyl carbonate	204-503-8	121-88-0	121880	1737	Reach_1021	1365	3.88	0.61	3				-4.8	-5.4	-7.1	0.0%	0.0%	0.0%
ferrate(4-), hexakis(cyano-C)-, Et 2-[6-(ethylamino)-3-(ethiminc	223-772-2	4065-45-6	4065456	52	Reach_2009	1366	6.61	0.69	4	5.61	0.69		-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
benz[cd]indol-2(1H)-one	228-168-2	6153-05-5	6153055	1279	Reach_2154	1367	3.56	1.09	3				-4.8	-5.4	-7.1	0.0%	0.0%	0.0%
611-813-0	229-653-1	6640-22-8	6640228	5979	Reach_2199	1368							-5.6	-5.4	-7.1	0.0%	0.0%	0.0%
619-518-9	700-349-5	33719-11-8	33719118	5849	Reach_4871	1369	4.45		1				-4.8	-5.4	-7.1	0.0%	0.0%	0.0%
[4-[p,p'-bis(dimethylamino)benzhydrylidene]cyclohexa-2,5-dien-	265-449-9	65113-55-5	65113555	5970	Reach_2868	1370	0.83		2				-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
2,2-bis(hydroxymethyl)propionic acid	225-306-3	4767-03-7	4767037	1272	Reach_2063	1371	5.88		1				-4.4	-5.4	-7.1	0.0%	0.0%	0.0%
605-866-9	609-962-1	41851-59-6	41851596	2884	Reach_4317	1372	4.72		1				-4.7	-5.4	-7.1	0.0%	0.0%	0.0%
disodium 4,4'-bis[[4-anilino-6-[(2-hydroxyethyl)amino]-1,3,5-tria	267-400-7	67859-51-2	67859512	5989	Reach_2892	1373	5.46	0.72	3	4.44	0.82		-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
chloroethane	200-830-5	75-00-3	75003	3654	Reach_122	1374	4.99	0.15	3	3.99	0.15		-5.8	-5.4	-7.4	0.0%	0.0%	0.0%
1,4-dioxacycloheptadecane-5,17-dione	203-347-8	105-95-3	105953	1422	Reach_652	1375	3.46	0.42	3	2.46	0.42		-5.1	-5.4	-6.9	0.0%	0.0%	0.0%
oxybenzone	205-031-5	131-57-7	131577	22	Reach_1122	1376	3.42	0.53	3	2.65	0.50		-5.4	-5.4	-6.5	0.0%	0.0%	0.0%
[[(phosphonomethyl)imino]bis[hexamethylenenitrilobis(methyle	252-156-6	34690-00-1	34690001	2714	Reach_2680	1377	5.41	0.29	3	4.41	0.29		-4.6	-5.4	-7.0	0.0%	0.0%	0.0%
diammonium [[N,N'-ethylenebis[N-(carboxylatomethyl)glycinatc	241-883-4	17958-73-5	17958735	5745	Reach_2449	1378	5.68		1	4.16			-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
2,6-difluorobenzamide	202-150-4	92-36-4	92364	4032	Reach_384	1379	5.50		1				-5.3	-5.4	-7.1	0.0%	0.0%	0.0%
2,6-dichloro-4,8-dipiperidinopyrimido[5,4-d]pyrimidine	613-175-9	6318-09-8	6318098	1282	Reach_4383	1380	4.24	0.29	3	2.78	0.82		-5.0	-5.4	-6.7	0.0%	0.0%	0.0%
barbituric acid	200-658-0	67-52-7	67527	3495	Reach_83	1381	5.38	1.80	3				-4.4	-5.4	-7.1	0.0%	0.0%	0.0%
peracetic acid	201-186-8	79-21-0	79210	917	Reach_235	1382	2.94	0.67	3	2.40	0.80		-5.6	-5.4	-6.9	0.0%	0.0%	0.0%
(2S)-[(tert-butoxycarbonyl)amino](3-hydroxytricyclo[3.3.1.13,7]c	700-361-0	361442-00-4	361442004	2760	Reach_4874	1383	4.65		1				-4.9	-5.4	-7.1	0.0%	0.0%	0.0%
3-ethoxy-4-hydroxybenzaldehyde	204-464-7	121-32-4	121324	368	Reach_1010	1384	5.13	0.33	5	4.31	0.47		-5.1	-5.4	-7.0	0.0%	0.0%	0.0%
diisopropyl ether	203-560-6	108-20-3	108203	232	Reach_733	1385	5.85	0.59	7	4.85	0.70		-5.7	-5.4	-7.2	0.0%	0.0%	0.0%
icosyl acrylate	200-424-8	59-42-7	59427	3275	Reach_50	1386	3.66		1				-5.5	-5.4	-6.4	0.0%	0.0%	0.0%
N,N-dimethyl-p-toluidine	202-805-4	99-97-8	99978	1094	Reach_544	1387	4.41	0.18	5	3.41	0.18		-5.6	-5.4	-6.3	0.0%	0.0%	0.0%
isophthaloyl dichloride	202-774-7	99-63-8	99638	4214	Reach_535	1388	6.03	0.79	3	5.03	0.79		-5.6	-5.4	-7.0	0.0%	0.0%	0.0%
tributylmethylammonium chloride	260-135-8	56375-79-2	56375792	5935	Reach_2815	1389	4.03		1				-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
disodium 4-amino-3,6-bis[[4-[(2,4-diaminophenyl)azo]phenyl]azo	229-208-1	6428-31-5	6428315	5967	Reach_2185	1390	5.02		2				-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
4'-chloro-2',5'-dimethoxyacetoacetanilide	224-638-6	4433-79-8	4433798	2922	Reach_2035	1391	4.33		2				-4.7	-5.4	-7.0	0.0%	0.0%	0.0%
[nitrilotris(methylene)]trisphosphonic acid, ammonium salt	603-981-9	136890-12-5	136890125	1903	Reach_4135	1392	1.16	0.69	3				-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
1-hydroxy-4-methyl-6-(2,4,4-trimethylpentyl)pyridin-2(1H)-one,	202-874-0	100-64-1	100641	135	Reach_566	1393	4.88	0.54	4	3.16	0.66		-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
sodium 2-amino-4,6-dinitrophenoxide	203-960-0	112-33-4	112334	1583	Reach_898	1394	5.61	0.17	3	4.61	0.17		-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
hexamethylene diacrylate	235-921-9	13048-33-4	13048334	1837	Reach_2320	1395	3.53	0.31	3	2.53	0.31		-5.6	-5.4	-6.7	0.0%	0.0%	0.0%
potassium O-ethyl dithiocarbonate	203-552-2	108-12-3	108123	1476	Reach_730	1396	4.34	0.78	3	4.15	0.79		-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
N-(2-ethylhexyl)-1-[[2-methyl-4-[(2-methylphenyl)azo]phenyl]az	204-436-4	120-93-4	120934	367	Reach_1006	1397	6.52	1.15	6	5.52	1.15		-5.6	-5.4	-5.8	0.0%	0.0%	0.0%
(3R)-3-amino-1-[3-(trifluoromethyl)-5,6-dihydro[1,2,4]triazolo[4,	213-063-6	921-03-9	921039	4027	Reach_1591	1398	2.08		1				-4.9	-5.4	-6.7	0.0%	0.0%	0.0%
608-591-2	608-591-2	31221-06-4	31221064	5838	Reach_4279	1399							-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
zinc distearate	209-151-9	557-05-1	557051	5933	Reach_1371	1400	2.89	0.14	3	2.39	0.34		-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
Methyl 3-cyclopentyl-1-methyl-1H-indole-6-carboxylate	700-133-0	2436-29-5	2436295	2389	Reach_4774	1401	4.39	1.19	3				-5.5	-5.4	-6.9	0.0%	0.0%	0.0%
sodium N-(2-carboxyethyl)-N-dodecyl-β-alaninate	203-650-5	109-13-7	109137	1494	Reach_771	1402	4.27	0.72	3	3.27	0.72		-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
pent-1-ene	203-694-5	109-67-1	109671	1506	Reach_784	1403	4.75		2				-5.7	-5.4	-7.9	0.0%	0.0%	0.0%

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Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
ampicillin	239-477-7	15458-48-7	15458487	2037	Reach_2388	1404	4.95	1.51	3				-4.9	-5.4	-6.6	0.0%	0.0%	0.0%
2-ethoxyethanol	203-804-1	110-80-5	110805	284	Reach_829	1405	6.89	0.12	4	6.17	0.58		-5.6	-5.4	-7.0	0.0%	0.0%	0.0%
2-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol	274-570-6	70321-86-7	70321867	3559	Reach_2916	1406	1.06	0.46	3				-5.1	-5.4	-6.9	0.0%	0.0%	0.0%
[1-(4-bromobenzyl)-2-butyl-4-chloro-1H-imidazol-5-yl]methanol	604-770-4	151012-31-6	151012316	2016	Reach_4162	1407	3.27	0.62	3				-5.0	-5.4	-7.0	0.0%	0.0%	0.0%
dilactide	202-468-3	95-96-5	95965	4140	Reach_448	1408	5.75	0.50	3	5.14	0.48		-4.7	-5.4	-7.0	0.0%	0.0%	0.0%
aminoguanidinium hydrogen carbonate	219-956-7	2582-30-1	2582301	5800	Reach_1842	1409	5.29	1.22	3	4.29	1.22		-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
N-[3-(isodecyloxy)propyl]propane-1,3-diamine	276-432-0	72162-46-0	72162460	3598	Reach_2934	1410	3.27	0.57	3				-5.7	-5.4	-6.7	0.0%	0.0%	0.0%
trizinc dicitrate	208-901-2	546-46-3	546463	5926	Reach_1355	1411	4.61	2.53	3	3.61	2.53		-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
3,5,5-trimethylhexanal	226-603-0	5435-64-3	5435643	3140	Reach_2112	1412	4.39	0.34	3	3.39	0.34		-5.7	-5.4	-7.4	0.0%	0.0%	0.0%
pentane-1,2-diol	226-285-3	5343-92-0	5343920	3102	Reach_2100	1413	6.66	0.53	3	5.66	0.53		-5.2	-5.4	-7.0	0.0%	0.0%	0.0%
4-amino-5-methoxy-N,2-dimethylbenzenesulphonamide	203-040-9	102-56-7	102567	1345	Reach_593	1414	5.52		1				-4.7	-5.4	-7.0	0.0%	0.0%	0.0%
1,1'-binaphthyl-8,8'-dicarboxylic acid	700-688-9	111360-16-8	111360168	297	Reach_4968	1415	4.22	0.35	3				-5.2	-5.4	-6.8	0.0%	0.0%	0.0%
604-759-4	604-759-4	150928-21-5	150928215	2015	Reach_4161	1416	3.93	1.03	3				-4.7	-5.4	-7.0	0.0%	0.0%	0.0%
5-difluoromethoxy-2-[[(3,4-dimethoxy-2-pyridyl)methyl]thio]-1H	700-086-6	3159-04-4	3159044	1258	Reach_4756	1417	2.98	0.56	3				-4.9	-5.4	-7.0	0.0%	0.0%	0.0%
4,4'-azo-3-hydroxynaphthalene-1-sulphonate	600-593-1	104632-26-0	104632260	1396	PharmaBeta_621	1418	5.07		1				-4.5	-5.4	-7.0	0.0%	0.0%	0.0%
2-Methoxy-6-methylbenzoic acid	612-182-4	6161-65-5	6161655	3342	Reach_4373	1419	4.72	0.65	3				-4.8	-5.4	-7.0	0.0%	0.0%	0.0%
4-acetylmorpholine	216-913-4	1696-20-4	1696204	2118	Reach_1709	1420	6.41	0.91	3	5.41	0.91		-4.5	-5.4	-7.1	0.0%	0.0%	0.0%
{[2-(trifluoromethyl)benzoyl]amino}methyl acetate	619-484-5	895525-72-1	895525721	3978	Reach_4523	1421	3.77	0.68	3				-5.6	-5.4	-6.9	0.0%	0.0%	0.0%
pleuromulin	204-747-5	125-65-5	125655	1799	Reach_1084	1422	4.07	0.70	3				-4.8	-5.4	-7.0	0.0%	0.0%	0.0%
5-nitroisophthalic acid	210-568-3	618-88-2	618882	3358	Reach_1440	1423	6.23	0.57	3	5.23	0.57		-4.7	-5.4	-7.2	0.0%	0.0%	0.0%
2-(2-butoxyethoxy)ethyl 6-propylpiperonyl ether	200-076-7	51-03-6	51036	667	Reach_12	1424	3.44	0.55	32	2.42	0.55	6	-5.6	-5.4	-6.9	0.0%	0.0%	0.0%
2,2'-oxybis[5,5-dimethyl-1,3,2-dioxaphosphorinane] 2,2'-disulphi	223-829-1	4090-51-1	4090511	2866	Reach_2012	1425	5.39		3	4.39			-5.6	-5.4	-6.8	0.0%	0.0%	0.0%
methyl 3-mercaptopropionate	220-912-4	2935-90-2	2935902	2563	Reach_1888	1426	3.14	0.71	3	2.14	0.71		-5.6	-5.5	-6.9	0.0%	0.0%	0.0%
2-{[(4-chloro-3-methoxypyridin-2-yl)methyl]sulfanyl}-6-(difluoro	218-370-9	2135-17-3	2135173	532	Reach_1760	1427	5.00		3	4.00			-5.0	-5.5	-7.0	0.0%	0.0%	0.0%
4-(6-methylbenzothiazol-2-yl)aniline	207-141-9	443-83-4	443834	2924	Reach_1275	1428	3.86	0.11	3				-5.0	-5.5	-7.1	0.0%	0.0%	0.0%
ethane-1,2-diyl palmitate	210-826-5	624-03-3	624033	3368	Reach_1451	1429	4.36	1.15	3	3.36	1.15		-5.6	-5.5	-5.3	0.0%	0.0%	0.0%
sodium 1H-benzotriazolide	239-269-6	15217-42-2	15217422	5711	Reach_2379	1430	4.94	0.39	3	3.97	0.51		-5.2	-5.5	-6.8	0.0%	0.0%	0.0%
2-ethylhexyl 4-methoxycinnamate	226-775-7	5466-77-3	5466773	3151	Reach_2117	1431	4.40	1.73	3	3.40	1.73		-5.6	-5.5	-6.7	0.0%	0.0%	0.0%
2,4,6-trimethylbenzoyl chloride	208-235-2	517-23-7	517237	3044	Reach_1321	1432	5.68		2				-5.7	-5.5	-6.6	0.0%	0.0%	0.0%
1-methylimidazole	200-540-9	62-54-4	62544	6274	PharmaBeta_363	1433	6.22	0.24	3	5.22	0.24		-5.6	-5.5	-6.9	0.0%	0.0%	0.0%
2,5-dimethylhexyne-2,5-diol	700-314-4	82966-34-5	82966345	3838	Reach_4856	1434	3.92	0.33	3				-4.7	-5.5	-7.0	0.0%	0.0%	0.0%
Methyl 4-(butylamino)benzoate	629-348-7	23357-52-0	23357520	2350	Reach_4591	1435	4.25		1				-5.0	-5.5	-7.1	0.0%	0.0%	0.0%
N-phenylmaleimide	203-604-4	108-67-8	108678	242	Reach_751	1436	4.12	0.70	28	3.12	0.70		-4.8	-5.5	-7.1	0.0%	0.0%	0.0%
N1-methyl-4-(methylsulfonyl)benzene-1,2-diamine	615-907-2	73097-51-5	73097515	3613	Reach_4418	1437	4.09	0.68	3				-4.6	-5.5	-7.1	0.0%	0.0%	0.0%
4-(Methylamino)-3-nitrobenzoic acid	249-050-7	28479-22-3	28479223	2533	Reach_2618	1438	3.72	0.60	3	2.67	0.86		-4.7	-5.5	-7.3	0.0%	0.0%	0.0%
2-methylaminoethanol	203-710-0	109-83-1	109831	1510	Reach_793	1439	4.72	0.33	4	3.72	0.33		-5.5	-5.5	-7.1	0.0%	0.0%	0.0%
EPTC (reach)	212-073-8	759-94-4	759944	869	Reach_1529	1440	3.96	0.46	29	3.33	0.72	8	-5.7	-5.5	-6.7	0.0%	0.0%	0.0%
639-566-4	639-566-4	165184-98-5	165184985	2096	Reach_4605	1441	3.09	0.68	3	2.09	0.68		-5.7	-5.5	-6.6	0.0%	0.0%	0.0%
2-(4-aminophenyl)-6-methylbenzothiazole-7-sulphonic acid	696-374-3	100930-72-1	100930721	1312	Reach_4716	1442	1.60	1.20	3				-4.6	-5.5	-7.1	0.0%	0.0%	0.0%
dimethyl malonate	203-597-8	108-59-8	108598	1486	Reach_749	1443	5.26	0.64	3	4.26	0.64		-5.6	-5.5	-7.0	0.0%	0.0%	0.0%
dimethylcarbamoyl chloride	202-810-1	100-01-6	100016	120	Reach_547	1444	4.67	0.84	32	3.67	0.84		-5.7	-5.5	-7.0	0.0%	0.0%	0.0%
didecylamine	214-312-1	1120-49-6	1120496	1571	Reach_1659	1445	0.70	0.61	3				-5.3	-5.5	-6.7	0.0%	0.0%	0.0%
689-404-1	607-145-4	227197-72-0	227197720	2337	Reach_4233	1446	4.69		2				-4.6	-5.5	-7.1	0.0%	0.0%	0.0%
tert-butyl-4-methoxyphenol	204-352-8	119-80-2	119802	357	Reach_987	1447	4.87	0.35	3	4.16	0.50		-5.2	-5.5	-6.8	0.0%	0.0%	0.0%
3,4-dihydro-2-methoxy-2H-pyran	202-797-2	99-88-7	99887	4221	Reach_541	1448	3.96	0.58	3	2.96	0.58		-5.7	-5.5	-6.8	0.0%	0.0%	0.0%
4-aminotoluene-3-sulphonic acid	201-831-3	88-44-8	88448	3956	Reach_323	1449	4.92	0.63	3	3.92	0.63		-4.4	-5.5	-7.3	0.0%	0.0%	0.0%
1H-2-Benzopyran-1,4(3H)-dione	616-178-3	75028-24-9	75028249	3656	Reach_4425	1450	4.31	0.83	3				-5.0	-5.5	-7.1	0.0%	0.0%	0.0%
ethyl 2-[3-formyl-4-(2-methylpropoxy)phenyl]-4-methyl-1,3-thia	256-376-3	49562-28-9	49562289	649	Reach_2761	1451	4.42	1.04	12	3.42	1.04		-5.1	-5.5	-7.1	0.0%	0.0%	0.0%
3-methyl-1-vinyl-1H-imidazolium methyl sulphate	222-294-1	3407-42-9	3407429	2689	Reach_1956	1452	4.26	0.33	3	3.26	0.33		-5.2	-5.5	-6.8	0.0%	0.0%	0.0%
N-isopropyl-N'-phenyl-p-phenylenediamine	202-969-7	101-72-4	101724	1326	Reach_581	1453	3.69	1.01	3	2.69	0.52		-5.0	-5.5	-7.2	0.0%	0.0%	0.0%
trisodium 6,6',6''-(1,3,5-triazine-2,4,6-triyltriimino)trihexanoate	700-292-6	135043-68-4	135043684	5672	Reach_4846	1454							-5.2	-5.5	-6.8	0.0%	0.0%	0.0%
octacos-1-ene	260-124-8	56358-09-9	56358099	3191	Reach_2813	1455	3.65		1				-5.7	-5.5	-5.7	0.0%	0.0%	0.0%
cyclohexanecarboxylic acid	202-711-3	98-89-5	98895	1078	Reach_523	1456	4.84		2				-5.3	-5.5	-7.0	0.0%	0.0%	0.0%
β-alanine	203-536-5	107-95-9	107959	1472	Reach_722	1457	5.22	1.11	3				-4.4	-5.5	-7.2	0.0%	0.0%	0.0%
methyl cyanoacetate	203-288-8	105-34-0	105340	1412	Reach_638	1458	5.92		2				-5.6	-5.5	-7.1	0.0%	0.0%	0.0%
acetaldehyde oxime	203-479-6	107-29-9	107299	218	Reach_703	1459	5.05	0.52	4	4.18	0.77		-5.7	-5.5	-6.6	0.0%	0.0%	0.0%
tris[4-(diethylamino)phenyl]methylium acetate	263-974-8	63157-72-2	63157722	5960	Reach_2856	1460	1.90	0.58	3	0.91	0.28		-5.2	-5.5	-6.8	0.0%	0.0%	0.0%
glycollic acid	201-180-5	79-14-1	79141	3766	Reach_232	1461	5.05	0.43	3	4.33	0.44		-4.5	-5.5	-7.1	0.0%	0.0%	0.0%
methyl chloroformate	201-187-3	79-22-1	79221	3768	Reach_236	1462	3.32	1.41	3	2.32	1.41		-5.7	-5.5	-7.1	0.0%	0.0%	0.0%
theophylline	600-476-5	1037184-07-8	1037184078	1377	Reach_4065	1463	2.80	0.21	3				-4.8	-5.5	-6.3	0.0%	0.0%	0.0%
ethyl acetoacetate	205-516-1	141-97-9	141979	459	Reach_1170	1464	5.60	0.19	4	4.60	0.19		-5.7	-5.5	-6.8	0.0%	0.0%	0.0%
methyl [(2S,3S)-4-chloro-3-hydroxy-1-phenylbutan-2-yl]carbama	700-854-0	256473-04-8	256473048	2441	Reach_5014	1465	4.22	0.33	3	3.22	0.33		-4.8	-5.5	-7.1	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
ethyl (2R)-2-hydroxy-4-phenylbutanoate	210-195-6	609-66-5	609665	3321	Reach_1416	1466	4.77		1				-4.9	-5.5	-7.1	0.0%	0.0%	0.0%
ethyl 2-ethoxy-1-{[2'-(1H-tetrazol-5-yl)biphenyl-4-yl]methyl}-1H-	200-825-8	74-96-4	74964	843	Reach_119	1467	5.31	0.75	6	4.31	0.75		-5.0	-5.5	-7.1	0.0%	0.0%	0.0%
hexacos-1-ene	210-743-4	622-58-2	622582	3365	Reach_1446	1468	3.97	1.15	3	2.72	1.88		-5.7	-5.5	-6.1	0.0%	0.0%	0.0%
3,3'-[(2-chloro-5-methyl-p-phenylene)bis[imino(1-acetyl-2-oxoet	213-059-4	920-66-1	920661	1011	Reach_1590	1469	5.39		1				-5.2	-5.5	-6.4	0.0%	0.0%	0.0%
2-methyl-2-propylpropane-1,3-diol	249-942-6	29901-62-0	29901620	5827	Reach_2635	1470							-5.4	-5.5	-7.1	0.0%	0.0%	0.0%
1,2-benzisothiazol-3(2H)-one 1,1-dioxide	210-852-7	624-54-4	624544	3370	Reach_1453	1471	4.68	0.46	3	3.48	0.80		-5.1	-5.5	-6.4	0.0%	0.0%	0.0%
1,4-dimethoxy-2-nitrobenzene	201-903-4	89-39-4	89394	3973	Reach_342	1472	4.61		1				-5.7	-5.5	-7.1	0.0%	0.0%	0.0%
4-chloro-3,5-dinitro-α,α,α-trifluorotoluene	206-889-3	393-75-9	393759	2839	Reach_1265	1473	2.78		1				-5.7	-5.5	-6.8	0.0%	0.0%	0.0%
2-chloro-N,N-dimethyl-3-oxobutyramide	227-372-9	5810-11-7	5810117	1278	Reach_2137	1474	4.45		1				-4.7	-5.5	-7.0	0.0%	0.0%	0.0%
1,1'-dithiobis[hexahydro-2H-azepin-2-one]	250-056-7	30113-45-2	30113452	2586	Reach_2642	1475	3.04	0.64	3				-4.6	-5.5	-7.0	0.0%	0.0%	0.0%
1,4:3,6-dianhydro-D-glucitol	211-492-3	652-67-5	652675	3449	Reach_1488	1476	6.10	1.38	3				-4.8	-5.5	-7.2	0.0%	0.0%	0.0%
1,1-difluoroethylene	200-867-7	75-38-7	75387	3670	Reach_143	1477	5.32	0.13	3	4.32	0.13		-5.8	-5.5	-7.9	0.0%	0.0%	0.0%
606-738-5	200-709-7	69-53-4	69534	808	Reach_94	1478	4.84	2.09	7	3.84	2.09		-4.9	-5.5	-6.8	0.0%	0.0%	0.0%
3-amino-4-hydroxy-N-phenylbenzenesulphonamide	202-847-3	100-39-0	100390	1304	Reach_554	1479	3.81	1.09	3				-4.8	-5.5	-7.1	0.0%	0.0%	0.0%
diammonium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4	217-440-6	1852-04-6	1852046	2195	Reach_1726	1480	4.59		1				-5.2	-5.5	-6.8	0.0%	0.0%	0.0%
4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)pheny	233-215-5	10081-67-1	10081671	1310	Reach_2280	1481	5.00	0.12	3	4.00	0.12		-4.8	-5.5	-7.0	0.0%	0.0%	0.0%
5-ethyl-2-methylpyridine	203-250-0	104-90-5	104905	172	Reach_632	1482	4.77	0.75	8	3.09	0.75		-5.7	-5.5	-6.3	0.0%	0.0%	0.0%
607-936-4	224-339-0	4316-74-9	4316749	5886	Reach_2028	1483	7.24	1.03	3	6.24	1.03		-4.8	-5.5	-7.1	0.0%	0.0%	0.0%
8-isopropyl-8-azabicyclo[3.2.1]octan-3-one	620-037-1	99636-38-1	99636381	4213	Reach_4557	1484	4.26	1.47	3				-5.7	-5.5	-7.1	0.0%	0.0%	0.0%
methyl 2-naphthyl ether	202-213-6	93-04-9	93049	1017	Reach_397	1485	3.77	0.33	4	2.77	0.33		-5.7	-5.5	-6.4	0.0%	0.0%	0.0%
disodium (Z)-4-(9-octadecenylamino)-4-oxo-2(or 3)-sulphonatob	261-222-3	58353-68-7	58353687	5940	Reach_2828	1486	5.04	0.36	3	4.04	0.36		-5.2	-5.5	-6.8	0.0%	0.0%	0.0%
5,12-dihydroquino[2,3-b]acridine-7,14-dione	213-879-2	1047-16-1	1047161	1400	Reach_1636	1487	5.18	0.72	3	4.18	0.72		-4.9	-5.5	-7.1	0.0%	0.0%	0.0%
611-622-2	616-212-7	75330-75-5	75330755	856	Reach_4428	1488	4.31		1				-4.7	-5.5	-7.1	0.0%	0.0%	0.0%
2-[(4-chloro-2-nitrophenyl)azo]-N-(2,3-dihydro-2-oxo-1H-benzim	235-462-4	12236-62-3	12236623	1747	Reach_2307	1489	4.17	1.01	3	3.17	1.01		-4.9	-5.5	-7.2	0.0%	0.0%	0.0%
trimethyloctadecylammonium chloride	203-929-1	112-03-8	112038	5610	Reach_885	1490	1.71	0.24	3	0.71	0.24		-5.2	-5.5	-6.8	0.0%	0.0%	0.0%
619-682-1	211-932-4	713-95-1	713951	3581	Reach_1521	1491	4.45	0.77	3	3.45	0.77		-4.8	-5.5	-6.8	0.0%	0.0%	0.0%
2-hexyloxyethanol	203-951-1	112-25-4	112254	1580	Reach_893	1492	5.18	0.18	3	4.17	0.37		-5.7	-5.5	-7.0	0.0%	0.0%	0.0%
618-965-7	616-640-4	78628-80-5	78628805	6038	Reach_4442	1493	1.78		2				-4.7	-5.5	-7.1	0.0%	0.0%	0.0%
O-(4-bromo-2-chlorophenyl) O-ethyl S-propyl phosphorothioate	217-983-9	2031-67-6	2031676	2259	Reach_1746	1494	6.25	1.08	3	5.22	0.77		-5.6	-5.5	-6.4	0.0%	0.0%	0.0%
(carboxymethyl)dimethyl-3-[(1-oxododecyl)amino]propylammor	224-292-6	4292-10-8	4292108	1267	Reach_2026	1495	3.57	0.44	3	2.86	0.55		-4.9	-5.5	-7.1	0.0%	0.0%	0.0%
lithium 2-methoxy-4-(trifluoromethyl)pyridine-3-thiolate	617-976-4	871544-06-8	871544068	6072	Reach_4483	1496							-5.2	-5.5	-6.8	0.0%	0.0%	0.0%
606-819-5	606-819-5	216699-04-6	216699046	5773	Reach_4219	1497	5.30	0.25	3	4.30	0.25		-5.2	-5.5	-6.8	0.0%	0.0%	0.0%
2,2'-[ethylenebis(oxyphenyl-2,1-eneazo)]bis[N-(2,3-dihydro-2-ox	278-770-4	77804-81-0	77804810	3736	Reach_2951	1498	4.17	1.01	3	3.17	1.01		-5.9	-5.5	-7.0	0.0%	0.0%	0.0%
benzonitrile	202-855-7	100-47-0	100470	128	Reach_560	1499	4.91	0.70	28	3.91	0.70		-5.7	-5.5	-6.6	0.0%	0.0%	0.0%
4-nitro-o-anisidine	202-588-6	97-52-9	97529	4165	Reach_479	1500	4.36	0.45	3	3.36	0.45		-4.8	-5.5	-7.2	0.0%	0.0%	0.0%
(4R,6R)-4-Hydroxy-2,2,6-trimethylcyclohexanone	700-220-3	99636-32-5	99636325	4212	Reach_4808	1501	4.26	1.47	3				-5.2	-5.5	-7.1	0.0%	0.0%	0.0%
3-(4-methyl-1H-imidazol-1-yl)-5-(trifluoromethyl)aniline	255-848-6	42487-72-9	42487729	2894	Reach_2751	1502	5.43		2				-4.9	-5.5	-7.1	0.0%	0.0%	0.0%
erythromycin	204-040-1	114-07-8	114078	336	Reach_933	1503	4.19	1.35	17	2.15	2.09	11	-4.9	-5.5	-6.9	0.0%	0.0%	0.0%
sodium 2-(2-dodecyloxyethoxy)ethyl sulphate	221-416-0	3088-31-1	3088311	5836	Reach_1914	1504	4.84	0.54	3	3.84	0.54		-5.2	-5.5	-6.8	0.0%	0.0%	0.0%
N-bromosuccinimide	204-877-2	128-08-5	128085	1815	Reach_1106	1505	2.81		1				-4.6	-5.5	-7.3	0.0%	0.0%	0.0%
3-(trimethoxysilyl)propiononitrile	224-207-2	4246-51-9	4246519	2893	Reach_2022	1506	5.25	0.55	3	4.25	0.55		-5.7	-5.5	-6.9	0.0%	0.0%	0.0%
trimethoxyvinylsilane	220-449-8	2768-02-7	2768027	1255	Reach_1864	1507	5.50	0.69	3	4.04	1.00		-5.7	-5.5	-7.1	0.0%	0.0%	0.0%
cetrimonium bromide	200-311-3	57-09-0	57090	1223	Reach_36	1508	2.10	0.80	11	1.37	0.70	16	-5.2	-5.5	-6.8	0.0%	0.0%	0.0%
4,4'-methylene bis(dibutyldithiocarbamate)	233-593-1	10254-57-6	10254576	1344	Reach_2285	1509	2.17	0.14	3	1.17	0.14		-5.1	-5.5	-7.0	0.0%	0.0%	0.0%
3,3'-[(2-chloro-5-methyl-p-phenylene)bis[imino(1-acetyl-2-oxoet	941-126-4	1499193-66-6	1499193666	5706	Reach_5178	1510							-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
methyl decanoate	203-766-6	110-42-9	110429	1520	Reach_813	1511	3.91	1.42	3	2.91	1.42		-5.7	-5.5	-7.1	0.0%	0.0%	0.0%
4,4',4''-(1-methylpropanyl-3-ylidene)tris[6-tert-butyl-m-cresol]	217-420-7	1843-03-4	1843034	2190	Reach_1724	1512	6.17	0.58	3	5.17	0.58		-5.7	-5.5	-5.8	0.0%	0.0%	0.0%
potassium sodium hydrogen 7-[{2-acetamido-4-[(4-ammonio-5-s	283-810-9	84713-17-7	84713177	3874	Reach_2977	1513	5.15	0.39	3	4.15	0.39		-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
tert-butyl (6S)-6-[4-(7-{2-[(1R,3S,4S)-2-(tert-butoxycarbonyl)-2-a	601-507-5	118135-28-7	118135287	1666	Reach_4092	1514	3.65	0.22	3	2.48	0.41		-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
sodium hydrogen 3-{[4-({4-[(2-aminopropyl)amino]-6-chloro-1,3,	617-708-6	85390-94-9	85390949	3886	Reach_4472	1515	3.00		1				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
2-[(1R,3S,4S)-2-azabicyclo[2.2.1]hept-3-yl]-5-(7-{2-[(6S)-5-azaspi	696-357-0	1182822-31-6	1182822316	1667	Reach_4715	1516	3.55	0.32	3				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
disodium [7-amino-4-(hydroxy-kO)-3-[(2-{[2-(hydroxy-kO)-5-sulf	220-098-0	2627-86-3	2627863	2461	Reach_1848	1517	4.27	0.21	3	3.27	0.21		-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
trisodium [2-[[α-[(3-amino-2-hydroxy-5-sulphophenyl)azo]benzy	204-376-9	120-20-7	120207	1706	Reach_991	1518	4.11	0.87	3				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
trisodium 7-[[4-[(4-aminophenyl)azo]phenyl]azo]naphthalene-1,	617-345-3	82543-14-4	82543144	3827	Reach_4453	1519	3.64	0.24	3				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
benzyl benzoate	204-402-9	120-51-4	120514	359	Reach_996	1520	3.21	0.57	4	2.40	0.55		-5.7	-5.5	-6.9	0.0%	0.0%	0.0%
Trisodium 2-[(E)-(6-amino-1-hydroxy-3-sulfonato-2-naphthyl)dia	917-818-7	73344-75-9	73344759	3620	Reach_5084	1521	3.99	0.66	3				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
617-589-0	615-749-4	72291-30-6	72291306	3601	Reach_4416	1522	1.55	4.80	3				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
Trisodium 2-[(E)-(6-amino-1-hydroxy-3-sulfonato-2-naphthyl)dia	607-929-6	26391-06-0	26391060	2467	Reach_4253	1523	4.48	1.55	3				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
805-364-1	302-748-6	94133-84-3	94133843	6088	Reach_3006	1524							-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
Trisodium 2-[(6-amino-1-hydroxy-3-sulfonato-2-naphthyl)diazen	260-591-8	57144-06-6	57144066	3226	Reach_2824	1525	3.02	0.82	3				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
N,N'-diisopropylethane-1,2-diaminium bis[(2R,3Z,5R)-3-(2-hydro	212-658-8	838-88-0	838880	3851	Reach_1563	1526	4.68		2				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
disodium 5-amino-4-hydroxy-3-[(2-hydroxy-5-nitrophenyl)azo]na	210-789-5	623-36-9	623369	3366	Reach_1449	1527	4.76	0.10	3	3.76	0.10		-5.2	-5.5	-6.9	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
(4S,4aS,5aR,12aS)-9-amino-4,7-bis(dimethylamino)-3,10,12,12a-	214-868-5	1203-17-4	1203174	1709	Reach_1673	1528	2.81	0.09	3				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
disodium 3-[[2-(acetylamino)-4-aminophenyl]azo]naphthalene-1	615-309-1	7159-96-8	7159968	3585	Reach_4414	1529	3.62	0.48	3				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
601-093-6	601-093-6	111453-32-8	111453328	1548	Reach_4078	1530	4.50	0.60	3	5.48			-4.7	-5.5	-7.1	0.0%	0.0%	0.0%
Sodium hydrogen 4-amino-2-{[1-ethyl-2-hydroxy-4-methyl-6-oxo	225-472-7	4866-00-6	4866006	2975	Reach_2065	1531	6.20		1				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
613-004-8	254-301-9	39118-50-8	39118508	2835	Reach_2723	1532	5.36	0.86	3				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
2-[2-(dimethylamino)ethoxy]ethanol	216-940-1	1704-62-7	1704627	2119	Reach_1710	1533	5.48	0.38	3	4.48	0.38		-5.1	-5.5	-7.2	0.0%	0.0%	0.0%
1,3-Thiazol-5-ylmethyl [(2R,5R)-5-amino-1,6-diphenylhexan-2-yl]	700-597-4	1215841-86-3	1215841863	1729	Reach_4945	1534	5.50		3	4.50			-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
sodium hydrogen 2-({4-[(2-aminopropyl)amino]-6-fluoro-1,3,5-tr	619-846-2	123989-28-6	123989286	1779	Reach_4549	1535	3.75		2				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
Ammonium (3R,5R)-3,5-dihydroxy-7-[(1S,2S,6S,8S,8aR)-6-hydrox	201-379-7	81-83-4	81834	3815	Reach_279	1536	6.54		1				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
barium bis(2-ethylhexanoate)	941-128-5	1499193-67-7	1499193677	5707	Reach_5179	1537							-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
2-{2-[4-(dibenzo[b,f][1,4]thiazepin-11-yl)piperazin-1-yl]ethoxy}et	602-964-3	123989-29-7	123989297	1780	Reach_4108	1538	3.67		2				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
Sodium 2-[(E)-(4-ammonio-2,5-dimethylphenyl)diazenyl]benzen	688-501-6	21700-31-2	21700312	2303	Reach_4645	1539	4.90		1				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
3,3'-dichloro[1,1'-biphenyl]-4,4'-bis(diazonium) dichloride	212-946-3	885-82-5	885825	3960	Reach_1584	1540	3.85	0.17	3				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
613-879-6	279-356-6	79953-85-8	79953858	6406	Reach_2958	1541	5.37	0.23	3	4.37	0.23		-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
3-ethoxypropylamine	211-951-8	719-80-2	719802	3596	Reach_1523	1542	4.50		1				-5.7	-5.5	-6.7	0.0%	0.0%	0.0%
α,α-diphenylpiperidine-4-methanol hydrochloride	605-954-7	181997-71-7	181997717	2173	Reach_4185	1543	3.67	0.25	3				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
608-782-0	248-576-4	27619-89-2	27619892	2513	Reach_2610	1544	3.66	0.28	3				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
pentasodium 2-{[8-({4-fluoro-6-[(4-{[2-(sulfonatooxy)ethyl]sulfor	612-957-7	62211-93-2	62211932	5954	Reach_4377	1545							-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
octocrilene	228-250-8	6197-30-4	6197304	3360	Reach_2157	1546	4.40	2.11	3	3.40	2.11		-5.2	-5.5	-6.5	0.0%	0.0%	0.0%
Dibenzo[b,f][1,4]thiazepin-11-amine hydrochloride (1:1)	602-965-9	123989-31-1	123989311	1781	Reach_4109	1547	4.04		2				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
diammonium propylenebis(dithiocarbamate)	215-863-0	1435-71-8	1435718	1968	Reach_1680	1548	4.00		1				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
sodium 3-hydroxy-2-naphthoate	223-423-4	3886-69-9	3886699	2827	Reach_1997	1549	4.25	0.34	3	3.25	0.34		-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
611-210-2	248-479-7	27472-21-5	27472215	2509	Reach_2606	1550	2.87	0.32	3				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
nickel(2+) propionate	220-612-3	2835-68-9	2835689	2527	Reach_1873	1551	6.33		1				-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
2-amino-2-phenylbutyrate sodium	606-239-2	19130-96-2	19130962	2222	Reach_4199	1552	5.88	1.20	3				-5.2	-5.5	-6.8	0.0%	0.0%	0.0%
N-tert-butylglycyl chloride hydrochloride (1:1)	603-266-1	128286-13-5	128286135	1818	Reach_4113	1553	2.80	0.29	3				-5.2	-5.5	-6.8	0.0%	0.0%	0.0%
1-fluoro-4-nitrobenzene	206-502-8	350-46-9	350469	611	Reach_1242	1554	4.85	0.70	20	3.85	0.70		-5.7	-5.5	-6.5	0.0%	0.0%	0.0%
sodium 2-hexyloxyethanolate	206-566-7	354-64-3	354643	2738	Reach_1249	1555	4.08	0.20	3				-5.3	-5.5	-6.8	0.0%	0.0%	0.0%
612-957-7	679-514-8	154279-60-4	154279604	2034	Reach_4620	1556	3.74	1.70	3	2.74	1.70		-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
sodium 4-aminobenzoate	217-385-8	1830-54-2	1830542	2178	Reach_1723	1557	5.00		1				-5.3	-5.5	-6.8	0.0%	0.0%	0.0%
sodium anthranilate	605-991-9	183322-16-9	183322169	2184	Reach_4187	1558	3.98	0.78	3				-5.3	-5.5	-6.8	0.0%	0.0%	0.0%
602-891-7	602-891-7	122731-59-3	122731593	1758	Reach_4107	1559	4.62	0.14	3				-4.9	-5.5	-7.1	0.0%	0.0%	0.0%
sodium taurinate	219-265-0	2398-81-4	2398814	2363	Reach_1793	1560	5.24	0.76	3				-5.3	-5.5	-6.8	0.0%	0.0%	0.0%
ethyl glycinate hydrochloride	607-358-2	24338-09-8	24338098	2388	Reach_4239	1561	2.76	0.73	3				-5.3	-5.5	-6.8	0.0%	0.0%	0.0%
cyclohexane-1,3-dione, monosodium salt	606-440-5	201214-53-1	201214531	2251	Reach_4209	1562	4.11	1.09	3				-5.3	-5.5	-6.8	0.0%	0.0%	0.0%
anisaldehyde	204-602-6	123-11-5	123115	1763	Reach_1039	1563	5.00	0.15	3	4.13	0.33		-5.7	-5.5	-7.0	0.0%	0.0%	0.0%
sodium β-alaninate	692-511-6	63661-82-5	63661825	3416	Reach_4675	1564	4.12	0.43	3				-5.3	-5.5	-6.8	0.0%	0.0%	0.0%
O,O-dimethyl phosphorochloridothioate	219-754-9	2524-03-0	2524030	2424	Reach_1828	1565	4.67	0.39	3	3.67	0.39		-5.7	-5.5	-6.8	0.0%	0.0%	0.0%
N-methylacetamide	229-542-8	6600-31-3	6600313	3458	Reach_2195	1566	4.61	1.26	3	3.61	1.26		-5.2	-5.5	-7.0	0.0%	0.0%	0.0%
bis(2,4-dichlorophenyl) carbonate	247-748-6	26496-99-1	26496991	2471	Reach_2584	1567	3.75		1				-5.6	-5.5	-6.6	0.0%	0.0%	0.0%
but-2-ene-1,4-diol	212-472-7	821-06-7	821067	3818	Reach_1553	1568	4.00		1				-4.9	-5.5	-7.1	0.0%	0.0%	0.0%
618-109-2	208-844-3	543-49-7	543497	3139	Reach_1350	1569	4.46	0.44	3				-5.7	-5.5	-6.8	0.0%	0.0%	0.0%
608-991-7	259-197-9	54527-65-0	54527650	3147	Reach_2800	1570	4.24	0.85	3				-5.7	-5.5	-6.8	0.0%	0.0%	0.0%
[3-(2,3-epoxypropoxy)propyl]triethoxysilane	220-011-6	2602-34-8	2602348	2449	Reach_1843	1571	5.39	0.12	3	4.39	0.12		-5.7	-5.5	-7.0	0.0%	0.0%	0.0%
Heptan-2-yl [(5-chloroquinolin-8-yl)oxy]acetate	619-447-3	99607-70-2	99607702	1089	Reach_4521	1572	3.94	0.91	11	3.33	1.32	4	-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
3-methylbutan-1-ol	204-633-5	123-51-3	123513	394	Reach_1051	1573	5.70	0.70	16	4.68	0.70		-5.7	-5.5	-6.5	0.0%	0.0%	0.0%
1,3,5-tris[[4-tert-butyl-3-hydroxy-2,6-xylyl]methyl]-1,3,5-triazine	254-996-9	40601-76-1	40601761	2859	Reach_2731	1574	4.53	2.58	3	3.53	2.58		-5.7	-5.5	-4.8	0.0%	0.0%	0.0%
triethoxy(vinyl)silane	201-081-7	78-08-0	78080	3746	Reach_193	1575	6.21	1.07	3	5.21	1.07		-5.7	-5.5	-7.0	0.0%	0.0%	0.0%
dimethyl 2,5-dioxocyclohexane-1,4-dicarboxylate	202-676-4	98-52-2	98522	1072	Reach_509	1576	4.43	0.40	3	3.43	0.40		-4.8	-5.5	-7.3	0.0%	0.0%	0.0%
1-[4-(1,1-dimethylethyl)phenyl]-3-(4-methoxyphenyl)propane-1,	274-581-6	70356-09-1	70356091	3560	Reach_2917	1577	3.24	2.48	3	2.24	2.48		-5.6	-5.5	-7.0	0.0%	0.0%	0.0%
endo-8-isopropyl-8-azabicyclo[3.2.1]octan-3-ol	640-387-9	61477-40-5	61477405	3335	Reach_4608	1578	4.40	0.50	3				-5.5	-5.5	-7.1	0.0%	0.0%	0.0%
amoxicillin	265-634-4	65212-77-3	65212773	5973	Reach_2871	1579	5.83		1				-4.9	-5.5	-6.9	0.0%	0.0%	0.0%
α-acetyl-γ-butyrolactone	700-856-1	1247119-31-8	1247119318	5639	Reach_5015	1580							-5.6	-5.5	-7.3	0.0%	0.0%	0.0%
succinonitrile	248-003-8	26787-78-0	26787780	574	Reach_2594	1581	4.87	1.55	5	3.87	1.29		-5.2	-5.5	-7.1	0.0%	0.0%	0.0%
N-[(tert-butoxy)carbonyl]-L-valine	250-196-9	30433-91-1	30433911	2597	Reach_2647	1582	4.11		1				-5.0	-5.5	-7.1	0.0%	0.0%	0.0%
4,4'-methylenebis[N,N-bis(2,3-epoxypropyl)aniline]	249-204-3	28768-32-3	28768323	2543	Reach_2623	1583	3.82	0.15	3	2.82	0.15		-4.9	-5.5	-7.2	0.0%	0.0%	0.0%
4-amino-6-chlorotoluene-3-sulphonic acid	201-837-6	88-51-7	88517	3959	Reach_326	1584	6.39	0.40	3	5.39	0.40		-4.5	-5.5	-7.1	0.0%	0.0%	0.0%
D-gluconic acid, compound with N,N''-bis(4-chlorophenyl)-3,12-c	203-157-5	103-90-2	103902	165	Reach_616	1585	5.22	0.81	9	2.11	1.11		-5.2	-5.5	-6.9	0.0%	0.0%	0.0%
691-232-7	691-232-7	474266-68-7	474266687	5894	Reach_4665	1586							-5.3	-5.5	-6.9	0.0%	0.0%	0.0%
acid D,L-aspart	216-431-4	1583-59-1	1583591	2061	Reach_1697	1587	3.92	0.53	3				-4.5	-5.5	-7.2	0.0%	0.0%	0.0%
600-709-0	246-014-2	24085-08-3	24085083	5789	Reach_2538	1588	4.30		1				-4.9	-5.5	-7.1	0.0%	0.0%	0.0%
608-880-3	606-067-8	18595-18-1	18595181	2199	Reach_4191	1589	4.50	0.53	3				-5.0	-5.5	-7.1	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
2'-ethoxy-3-hydroxy-2-naphthanilide	202-185-5	92-74-0	92740	4048	Reach_391	1590	2.87		1				-5.0	-5.5	-6.9	0.0%	0.0%	0.0%
demeclocycline hydrochloride	200-592-2	64-73-3	64733	5969	Reach_74	1591							-5.3	-5.5	-6.9	0.0%	0.0%	0.0%
D-(-)-α-phenylglycine	200-752-1	71-41-0	71410	820	Reach_102	1592	5.65	0.70	44	5.01	0.70		-4.4	-5.5	-7.2	0.0%	0.0%	0.0%
1,4-dioxane	204-661-8	123-91-1	123911	16	Reach_1060	1593	6.85	0.70	24	5.92	0.88		-5.8	-5.5	-6.7	0.0%	0.0%	0.0%
dibenzoyl-L-tartaric acid monohydrate	242-040-3	18156-74-6	18156746	2169	Reach_2453	1594	3.39	0.73	3				-5.0	-5.5	-7.1	0.0%	0.0%	0.0%
6-Fluorochromane-2-carboxylic acid	610-555-6	50650-75-4	50650754	3013	Reach_4332	1595	3.79		1				-5.0	-5.5	-7.1	0.0%	0.0%	0.0%
603-772-2	247-362-8	25953-19-9	25953199	2448	Reach_2572	1596	4.96	1.35	3				-4.9	-5.5	-7.1	0.0%	0.0%	0.0%
4-tert-butylcyclohexanol	203-137-6	103-71-9	103719	1378	Reach_612	1597	4.42	1.22	3	3.42	1.22		-5.7	-5.5	-6.6	0.0%	0.0%	0.0%
cyclohexane-1,3-dione	207-980-0	504-02-9	504029	3005	Reach_1303	1598	4.42		2				-4.8	-5.5	-7.1	0.0%	0.0%	0.0%
isobutyric acid	201-195-7	79-31-2	79312	919	Reach_239	1599	5.38	0.52	5	4.30	0.39		-5.3	-5.5	-7.1	0.0%	0.0%	0.0%
2-chloro-3-(dimethylamino)-N,N-dimethylprop-2-en-1-iminium h	280-445-7	83411-71-6	83411716	3845	Reach_2966	1600	4.50		1				-5.3	-5.5	-6.9	0.0%	0.0%	0.0%
N-(2-benzoyl-4-chlorophenyl)cyclopropanecarboxamide	200-453-6	60-09-3	60093	746	Reach_54	1601	2.95	0.29	4	1.95	0.29		-5.3	-5.5	-6.8	0.0%	0.0%	0.0%
607-327-3	609-368-2	3724-43-4	3724434	5864	Reach_4300	1602							-5.7	-5.5	-7.1	0.0%	0.0%	0.0%
4-methylanisole	203-253-7	104-93-8	104938	1403	Reach_634	1603	5.23	0.50	3	4.23	0.50		-5.8	-5.5	-7.2	0.0%	0.0%	0.0%
1,1,1-trifluoroethane	206-996-5	420-46-2	420462	2887	Reach_1269	1604	4.85		1				-5.8	-5.5	-7.4	0.0%	0.0%	0.0%
2-ethoxy-1-methylethyl acetate	259-370-9	54839-24-6	54839246	3154	Reach_2802	1605	5.38	0.24	3	4.38	0.24		-5.7	-5.5	-6.7	0.0%	0.0%	0.0%
bis(2-methylisouronium) sulphate	245-642-4	23410-40-4	23410404	2351	Reach_2531	1606	5.06	0.76	3	4.18	0.75		-5.3	-5.5	-6.9	0.0%	0.0%	0.0%
α-chloro-4-fluoroacetophenone	218-377-7	2136-89-2	2136892	2291	Reach_1761	1607	5.67		2				-5.7	-5.5	-6.9	0.0%	0.0%	0.0%
3,3'-oxybis(ethyleneoxy)bis(propylamine)	219-764-3	2526-62-7	2526627	2427	Reach_1830	1608	7.83	0.93	3	4.19	0.85		-4.7	-5.5	-7.3	0.0%	0.0%	0.0%
610-491-9	212-726-7	859-18-7	859187	1237	Reach_1567	1609	3.38	1.86	3	2.38	1.29		-5.2	-5.5	-7.1	0.0%	0.0%	0.0%
12-aminododecanoic acid	204-251-9	118-45-6	118456	1670	Reach_963	1610	6.40	0.19	3	5.40	0.19		-4.6	-5.5	-7.2	0.0%	0.0%	0.0%
3-aminobenzenesulphonic acid	204-473-6	121-47-1	121471	1728	Reach_1015	1611	5.13		2				-4.7	-5.5	-7.3	0.0%	0.0%	0.0%
dibutyltin di(acetate)	213-928-8	1067-33-0	1067330	199	Reach_1639	1612	2.48	0.72	5	1.48	1.06		-5.4	-5.5	-6.3	0.0%	0.0%	0.0%
2,2-dimethylpropan-1-ol, tribromo derivative	253-057-0	36483-57-5	36483575	2768	Reach_2700	1613	4.53	0.55	3	3.53	0.55		-5.7	-5.5	-7.1	0.0%	0.0%	0.0%
3-methyl-1-phenyl-5-pyrazolone	216-319-5	1558-33-4	1558334	2045	Reach_1690	1614	4.11		1				-4.9	-5.5	-7.1	0.0%	0.0%	0.0%
tetradecyl methacrylate	219-835-9	2549-53-3	2549533	2435	Reach_1835	1615	1.18	0.71	3	0.76			-5.5	-5.5	-7.1	0.0%	0.0%	0.0%
616-785-3	231-001-6	7400-27-3	7400273	6020	Reach_2249	1616							-4.9	-5.5	-7.1	0.0%	0.0%	0.0%
but-3-en-3-olide	211-617-1	674-82-8	674828	3493	Reach_1494	1617	5.46	0.24	3	4.46	0.24		-5.7	-5.5	-6.9	0.0%	0.0%	0.0%
piperidine	203-813-0	110-89-4	110894	289	Reach_836	1618	4.63	0.57	4	3.63	0.70		-5.7	-5.5	-6.7	0.0%	0.0%	0.0%
isovaleraldehyde	209-691-5	590-86-3	590863	733	Reach_1389	1619	4.48	0.72	4	4.20	0.28		-5.8	-5.5	-6.9	0.0%	0.0%	0.0%
bis(2-ethylhexyl) peroxydicarbonate	240-282-4	16111-62-9	16111629	2079	Reach_2413	1620	4.55	0.38	3	3.55	0.38		-5.2	-5.5	-6.5	0.0%	0.0%	0.0%
endo-(±)-8-aza-8-isopropylbicyclo[3.2.1]oct-3-yl (hydroxymethyl	606-548-2	204254-84-2	204254842	2263	Reach_4211	1621	4.67		2				-4.8	-5.5	-7.1	0.0%	0.0%	0.0%
4-tert-butylbenzaldehyde	213-367-9	939-97-9	939979	4095	Reach_1613	1622	3.53	0.85	3	2.65	0.78		-5.8	-5.5	-6.8	0.0%	0.0%	0.0%
hexahydro-1,3,5-tris(1-oxoallyl)-1,3,5-triazine	213-501-6	959-52-4	959524	4138	Reach_1619	1623	4.52	0.79	3				-4.6	-5.5	-7.4	0.0%	0.0%	0.0%
dimethyl isophthalate	215-951-9	1459-93-4	1459934	1990	Reach_1685	1624	4.38	0.39	3	3.46	0.54		-5.7	-5.5	-7.1	0.0%	0.0%	0.0%
trimethyl phosphite	204-471-5	121-45-9	121459	1727	Reach_1014	1625	6.08	0.39	3				-5.7	-5.5	-6.7	0.0%	0.0%	0.0%
hexadecyldimethylamine	203-997-2	112-69-6	112696	1598	Reach_919	1626	2.12	0.66	3	1.18	0.77		-5.6	-5.5	-7.4	0.0%	0.0%	0.0%
617-346-9	700-272-7	754186-36-2	754186362	6026	Reach_4832	1627							-4.9	-5.5	-7.1	0.0%	0.0%	0.0%
2-amino-6-fluorobenzonitrile	204-485-1	121-60-8	121608	1730	Reach_1017	1628	5.36	0.40	3	4.36	0.40		-5.7	-5.5	-7.1	0.0%	0.0%	0.0%
5-chloro-o-toluidine	258-907-4	53994-69-7	53994697	3116	Reach_2796	1629	4.51	1.89	3				-5.1	-5.5	-7.1	0.0%	0.0%	0.0%
606-722-8	212-786-4	869-24-9	869249	6071	Reach_1576	1630	4.79	0.47	3	3.79	0.47		-4.9	-5.5	-6.8	0.0%	0.0%	0.0%
N-[(1,1,3,3-tetramethylbutyl)phenyl]naphthalen-1-amine	257-406-8	51772-35-1	51772351	3046	Reach_2774	1631	4.18		1				-5.2	-5.5	-7.1	0.0%	0.0%	0.0%
1-(2,2-difluoro-1,3-benzodioxol-5-yl)cyclopropanecarboxylic acid	688-133-6	338-65-8	338658	2688	Reach_4641	1632	4.48	0.52	3				-5.1	-5.5	-7.1	0.0%	0.0%	0.0%
octan-2-ol	204-667-0	123-96-6	123966	399	Reach_1063	1633	4.61	0.27	3	3.61	0.27		-5.8	-5.5	-6.6	0.0%	0.0%	0.0%
hexa-2,4-dienoic acid	208-482-6	530-48-3	530483	3084	Reach_1326	1634	4.16		2				-5.0	-5.5	-7.2	0.0%	0.0%	0.0%
2-tert-butyl-p-cresol	219-314-6	2409-55-4	2409554	2373	Reach_1800	1635	3.26	0.19	3	2.26	0.19		-5.7	-5.5	-7.0	0.0%	0.0%	0.0%
prop-2-yn-1-ol	203-471-2	107-19-7	107197	214	Reach_698	1636	3.57	0.41	4	2.57	0.41		-5.7	-5.5	-7.0	0.0%	0.0%	0.0%
4-chloro-o-xylene	210-248-3	611-06-3	611063	755	Reach_1417	1637	3.54	0.54	5	3.06	0.70		-5.8	-5.5	-7.4	0.0%	0.0%	0.0%
4-chloro-α,α,α-trifluoro-o-toluidine	210-856-9	624-65-7	624657	3372	Reach_1454	1638	4.26		1				-5.4	-5.6	-7.2	0.0%	0.0%	0.0%
biphenyl	202-163-5	92-52-4	92524	1012	Reach_385	1639	3.39	0.70	36	2.40	0.22		-5.8	-5.6	-6.8	0.0%	0.0%	0.0%
hexafluoropropene	204-127-4	116-15-4	116154	1646	Reach_952	1640	4.83	0.29	3	3.83	0.29		-5.8	-5.6	-7.8	0.0%	0.0%	0.0%
trichloro(hexadecyl)silane	227-575-2	5894-60-0	5894600	3260	Reach_2142	1641	4.00		1				-5.4	-5.6	-6.1	0.0%	0.0%	0.0%
α-hydroxy-β,β-dimethyl-γ-butyrolactone	209-963-3	599-04-2	599042	3296	Reach_1408	1642	5.50	0.66	3	4.50	0.66		-4.7	-5.6	-7.3	0.0%	0.0%	0.0%
2-oxo-2-[(4aS,4bS,5aS,6aS,6bS,9aR,10aS,10bS)-4a,6a,8,8-tetram	607-542-2	25092-32-4	25092324	2414	Reach_4243	1643	4.40		2				-4.9	-5.6	-7.1	0.0%	0.0%	0.0%
bis(2-hydroxyethyl) (6H-dibenz[c,e][1,2]oxaphosphorin-6-ylmeth	264-313-6	63562-34-5	63562345	3405	Reach_2860	1644	4.11	0.43	3	3.11	0.43		-4.7	-5.6	-7.1	0.0%	0.0%	0.0%
O-(1-chloroethyl) S-methyl carbonothioate	700-190-1	91507-67-4	91507674	4016	Reach_4799	1645	4.01	0.85	3				-5.8	-5.6	-6.8	0.0%	0.0%	0.0%
4,6-diphenyl-1,3,5-triazin-2(1H)-one	222-374-6	3452-07-1	3452071	1261	Reach_1963	1646	6.38	0.27	3	5.38	0.27		-4.9	-5.6	-7.0	0.0%	0.0%	0.0%
sodium 1,4-diisotridecyl sulphonatosuccinate	619-547-7	211515-46-7	211515467	2284	Reach_4529	1647	4.14		2				-5.3	-5.6	-6.9	0.0%	0.0%	0.0%
2-aminobenzene-1,4-disulphonic acid	202-669-6	98-44-2	98442	4185	Reach_507	1648	5.04	0.74	3	4.04	0.74		-4.5	-5.6	-7.2	0.0%	0.0%	0.0%
1-ethylpiperazine	226-166-6	5308-25-8	5308258	3087	Reach_2096	1649	5.50	0.16	3	4.55	0.36		-5.7	-5.6	-7.2	0.0%	0.0%	0.0%
dipotassium hydrogen 7-aminonaphthalene-1,3,6-trisulphonate	284-333-9	84852-23-3	84852233	6054	Reach_2980	1650							-5.3	-5.6	-6.9	0.0%	0.0%	0.0%
4-methylpent-3-en-2-one	205-502-5	141-79-7	141797	1942	Reach_1169	1651	5.31	0.20	3	4.31	0.20		-5.8	-5.6	-6.9	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
2-methyl-3-phenylpropanol	221-639-3	3173-53-3	3173533	2630	Reach_1925	1652							-5.8	-5.6	-7.1	0.0%	0.0%	0.0%
phenylacetonitrile	609-997-2	42221-52-3	42221523	4319	Reach_4319	1653	5.62		1				-5.8	-5.6	-6.7	0.0%	0.0%	0.0%
609-997-2	617-843-0	86386-77-8	86386778	6063	Reach_4476	1654							-5.8	-5.6	-6.6	0.0%	0.0%	0.0%
7-hydroxycitronellal	203-518-7	107-75-5	107755	1468	Reach_714	1655	5.07	0.56	3	4.07	0.56		-5.6	-5.6	-7.1	0.0%	0.0%	0.0%
bornan-2-one	200-945-0	76-22-2	76222	872	Reach_175	1656	4.75	0.92	6	3.75	0.92		-5.8	-5.6	-7.0	0.0%	0.0%	0.0%
butan-2-one O,O',O''-(vinylsilylidyne)trioxime	218-747-8	2224-33-1	2224331	2325	Reach_1774	1657	5.51	1.07	3	3.94	0.83		-5.6	-5.6	-6.5	0.0%	0.0%	0.0%
4-methylmorpholine	203-640-0	109-02-4	109024	1493	Reach_769	1658	5.41	0.35	3	4.41	0.35		-5.7	-5.6	-7.1	0.0%	0.0%	0.0%
Propan-2-yl [(4R,6R)-6-{2-[2-(4-fluorophenyl)-3-phenyl-4-(phenyl	700-243-9	1112262-71-1	1112262711	1543	Reach_4818	1659	0.51	0.79	3				-5.0	-5.6	-7.0	0.0%	0.0%	0.0%
1-benzyl-3-carboxylatopyridinium sodium chloride	268-692-9	68133-60-8	68133608	5993	Reach_2897	1660							-5.3	-5.6	-6.9	0.0%	0.0%	0.0%
flufenamic acid	939-996-5	689294-28-8	689294288	3532	Reach_5162	1661	3.60	0.45	3				-5.1	-5.6	-7.1	0.0%	0.0%	0.0%
2-ethylhexyl mercaptoacetate	231-626-4	7659-86-1	7659861	3721	Reach_2267	1662	2.82	0.61	3	2.09	0.61		-5.8	-5.6	-8.1	0.0%	0.0%	0.0%
N,N-dimethyltetradecylamine N-oxide	222-059-3	3332-27-2	3332272	2679	Reach_1949	1663	3.28	0.92	3	2.49	0.43		-5.1	-5.6	-7.1	0.0%	0.0%	0.0%
3,3'-thiodi(propionic acid)	203-841-3	111-17-1	111171	1539	Reach_846	1664	4.77		2				-4.7	-5.6	-7.2	0.0%	0.0%	0.0%
2-[(2-acetamido-6,9-dihydro-6-oxo-1H-purin-9-yl]methoxy]ethyl	236-307-3	13290-96-5	13290965	1862	Reach_2328	1665	4.09	0.64	3				-4.5	-5.6	-7.2	0.0%	0.0%	0.0%
Methyl 2-amino-3-chlorobenzoate	607-917-0	263355-39-1	263355391	2465	Reach_4252	1666	4.15	0.78	3				-5.7	-5.6	-7.1	0.0%	0.0%	0.0%
2-(3-(4-amino-9,10-dihydro-3-sulpho-9,10-dioxoanthracen-4-yl)a	219-949-9	2580-78-1	2580781	5799	Reach_1841	1667	5.17	0.71	3	3.86	0.70		-5.3	-5.6	-6.9	0.0%	0.0%	0.0%
(E)-1,4-dibromobut-2-ene	606-728-0	212322-56-0	212322560	2287	Reach_4214	1668	4.60	0.76	3				-5.8	-5.6	-6.7	0.0%	0.0%	0.0%
salicylonitrile	210-259-3	611-20-1	611201	3327	Reach_1420	1669	4.46		2				-5.3	-5.6	-7.1	0.0%	0.0%	0.0%
disodium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4-)-N,	238-372-3	14402-88-1	14402881	5698	Reach_2365	1670	5.46	0.73	3	4.43	0.84		-5.3	-5.6	-6.9	0.0%	0.0%	0.0%
613-099-6	218-491-7	2163-00-0	2163000	2301	Reach_1768	1671	4.02	0.61	3	3.02	0.61		-5.3	-5.6	-7.0	0.0%	0.0%	0.0%
2-(3-chlorophenyl)-2,4-dihydro-5-methyl-3H-pyrazol-3-one	216-544-9	1609-86-5	1609865	2078	Reach_1699	1672							-5.0	-5.6	-7.1	0.0%	0.0%	0.0%
methyl trimethyl-3-[(1-oxododecyl)amino]propylammonium sul	234-204-8	10595-49-0	10595490	5596	Reach_2300	1673	4.33	2.16	3	3.33	2.16		-5.3	-5.6	-6.9	0.0%	0.0%	0.0%
1-[2-(dimethylamino)-1-(4-methoxyphenyl)ethyl]cyclohexanol	608-782-0	32765-81-4	32765814	5844	Reach_4282	1674							-5.3	-5.6	-6.6	0.0%	0.0%	0.0%
glycine	200-272-2	56-40-6	56406	3197	Reach_27	1675	5.29	1.14	3				-4.5	-5.6	-7.3	0.0%	0.0%	0.0%
octylphosphonic acid	225-218-5	4724-48-5	4724485	2964	Reach_2060	1676	4.63	0.39	3	3.63	0.39		-5.0	-5.6	-7.2	0.0%	0.0%	0.0%
2-(2-phenoxyethoxy)ethanol	257-093-8	51263-08-2	51263082	5904	Reach_2771	1677							-4.9	-5.6	-7.3	0.0%	0.0%	0.0%
2-nitrophenol	201-857-5	88-75-5	88755	988	Reach_332	1678	4.43	0.84	36	3.43	0.84		-5.8	-5.6	-6.5	0.0%	0.0%	0.0%
2-ethyl-4-methylimidazole	230-786-2	7320-37-8	7320378	3615	Reach_2236	1679	2.00	0.37	3				-5.6	-5.6	-7.1	0.0%	0.0%	0.0%
triclocarban	202-924-1	101-20-2	101202	143	Reach_574	1680	1.68	0.69	5	1.06	0.67		-5.2	-5.6	-6.3	0.0%	0.0%	0.0%
tetrahydrofurfuryl alcohol	202-625-6	97-99-4	97994	1062	Reach_493	1681	5.70	1.14	3	4.98			-5.7	-5.6	-7.2	0.0%	0.0%	0.0%
(S)-2-amino-3-(3,4-dimethoxyphenyl)-2-methylpropiononitrile m	202-594-9	97-61-0	97610	1058	Reach_482	1682	5.18		1				-5.3	-5.6	-6.9	0.0%	0.0%	0.0%
4-(methylthio)-3,5-xylenol	265-747-9	65405-84-7	65405847	3453	Reach_2873	1683	3.06		1				-5.7	-5.6	-7.1	0.0%	0.0%	0.0%
tert-butyl 3-(6-amino-3-methylpyridin-2-yl)benzoate	207-100-5	434-16-2	434162	2912	Reach_1273	1684	0.89	0.45	3				-5.1	-5.6	-7.1	0.0%	0.0%	0.0%
piperazine, compound with phosphoric acid	230-745-9	7300-34-7	7300347	3612	Reach_2235	1685	5.27	0.64	3	4.27	0.64		-5.3	-5.6	-6.9	0.0%	0.0%	0.0%
3,3,5-trimethylcyclohexanol	204-122-7	116-02-9	116029	1642	Reach_949	1686	4.72		2				-5.8	-5.6	-6.9	0.0%	0.0%	0.0%
7-methoxy-4,4-dimethyl-1H-2-benzopyran-1,3(4H)-dione	603-200-1	127337-60-4	127337604	5648	Reach_4112	1687							-5.8	-5.6	-7.1	0.0%	0.0%	0.0%
(1R)-1-(3-methoxyphenyl)ethanamine	618-965-7	937203-35-5	937203355	4081	Reach_4504	1688	3.15	3.02	3				-5.8	-5.6	-7.1	0.0%	0.0%	0.0%
(1S)-1-(4-methoxyphenyl)ethanamine	298-842-9	93839-71-5	93839715	4089	Reach_3001	1689	5.00		1				-5.8	-5.6	-7.1	0.0%	0.0%	0.0%
606-907-3	222-746-8	3598-16-1	3598161	5858	Reach_1975	1690							-5.8	-5.6	-7.1	0.0%	0.0%	0.0%
benzyldimethylamine	203-149-1	103-83-3	103833	164	Reach_615	1691	4.01	0.85	3	3.01	0.85		-5.8	-5.6	-6.7	0.0%	0.0%	0.0%
1-ethylpyrrolidin-2-one	220-250-6	2687-91-4	2687914	2489	Reach_1853	1692	5.67	0.31	3	4.67	0.31		-5.8	-5.6	-7.2	0.0%	0.0%	0.0%
diethyl [4-(prop-2-yn-1-yloxy)benzylidene]propanedioate	207-959-6	503-01-5	503015	3001	Reach_1301	1693	3.42	0.66	3				-5.8	-5.6	-7.1	0.0%	0.0%	0.0%
4-methylthiosemicarbazide	229-563-2	6610-29-3	6610293	3462	Reach_2197	1694	4.27	0.45	3	3.27	0.45		-4.7	-5.6	-7.2	0.0%	0.0%	0.0%
4'-methoxyacetophenone	689-404-1	96240-10-7	96240107	4142	Reach_4651	1695	5.42	1.37	3				-5.8	-5.6	-7.1	0.0%	0.0%	0.0%
N'-[3-(dimethylamino)propyl]-N,N-dimethylpropane-1,3-diamine	229-761-9	6711-48-4	6711484	3485	Reach_2203	1696	4.42	0.41	3	3.18	0.60		-5.6	-5.6	-7.2	0.0%	0.0%	0.0%
tridecanedioic acid	208-011-4	505-52-2	505522	3008	Reach_1308	1697	3.13	0.54	3				-5.2	-5.6	-7.2	0.0%	0.0%	0.0%
dimethyl acetylsuccinate	202-550-9	96-99-1	96991	4160	Reach_475	1698	4.23	0.35	3				-5.7	-5.6	-7.3	0.0%	0.0%	0.0%
tert-butyl perbenzoate	210-382-2	614-45-9	614459	3334	Reach_1424	1699	3.55	0.60	3	2.61	0.62		-5.8	-5.6	-6.9	0.0%	0.0%	0.0%
2-tert-butylphenol	201-807-2	88-18-6	88186	983	Reach_318	1700	3.56	0.84	16	2.56	0.84		-5.8	-5.6	-6.5	0.0%	0.0%	0.0%
bis(2-ethylhexyl) azelate	203-091-7	103-24-2	103242	1361	Reach_604	1701	1.34	0.57	3	1.80			-5.6	-5.6	-6.4	0.0%	0.0%	0.0%
3,4,5-trimethoxytoluene	229-239-0	6443-69-2	6443692	3435	Reach_2187	1702	3.07	1.38	3				-5.8	-5.6	-7.0	0.0%	0.0%	0.0%
isopropyl myristate	203-751-4	110-27-0	110270	1516	Reach_810	1703	5.11		2	5.00			-5.7	-5.6	-7.4	0.0%	0.0%	0.0%
(1E)-1-(methoxyimino)-1-(2,5,5-trimethyl-1,3-dioxan-2-yl)aceton	619-753-7	73611-02-6	73611026	3625	Reach_4542	1704	4.44		2				-5.8	-5.6	-7.1	0.0%	0.0%	0.0%
2-chloroacetamide	201-174-2	79-07-2	79072	3765	Reach_227	1705	4.06	0.26	3	3.37	0.41		-4.7	-5.6	-7.1	0.0%	0.0%	0.0%
3,6,7-trimethyloct-6-en-1-yn-3-ol	201-368-7	81-64-1	81641	3808	Reach_276	1706	1.64		1				-5.8	-5.6	-7.1	0.0%	0.0%	0.0%
thymidine	200-070-4	50-89-5	50895	3021	Reach_10	1707	5.50		3	4.50			-4.7	-5.6	-7.4	0.0%	0.0%	0.0%
hexamethyldisiloxane	203-492-7	107-46-0	107460	1463	Reach_709	1708	3.09	1.16	3	3.09	1.61		-6.0	-5.6	-7.8	0.0%	0.0%	0.0%
2,2'-p-phenylenedioxydiethanol	203-197-3	104-38-1	104381	1393	Reach_621	1709	6.19	0.43	3	5.19	0.43		-4.7	-5.6	-7.3	0.0%	0.0%	0.0%
629-935-8	629-935-8	32539-82-5	32539825	2654	Reach_4597	1710	3.19	1.20	3				-5.4	-5.6	-7.1	0.0%	0.0%	0.0%
bis(2-chloroethyl) ether	620-019-3	1124-64-7	1124647	5611	Reach_4556	1711							-5.8	-5.6	-6.7	0.0%	0.0%	0.0%
dihydrogen bis(acetato-O)difluoroborate(1-)	206-768-5	373-61-5	373615	5865	Reach_1260	1712	4.97	0.82	3	3.66	0.92		-5.3	-5.6	-6.9	0.0%	0.0%	0.0%
2,2'-azobis[2-methylbutyronitrile]	236-740-8	13472-08-7	13472087	1882	Reach_2338	1713	5.06	0.54	3	4.06	0.54		-5.8	-5.6	-7.0	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
dimethyl sulphide	200-846-2	75-18-3	75183	853	Reach_133	1714	4.66	0.50	4	3.66	0.50		-5.9	-5.6	-7.4	0.0%	0.0%	0.0%
N,N'-(2-chloro-5-methyl-1,4-phenylene)bis[3-oxobutyramide]	201-100-9	78-27-3	78273	893	Reach_197	1715	5.53	0.70	20	4.49	0.70		-4.8	-5.6	-7.1	0.0%	0.0%	0.0%
bis(pentane-2,4-dionato-O,O')bis(propan-2-olato)titanium	230-191-8	6969-71-7	6969717	3548	Reach_2216	1716	4.91		1				-5.3	-5.6	-7.0	0.0%	0.0%	0.0%
octanoyl chloride	203-891-6	111-64-8	111648	1551	Reach_862	1717	3.99	1.10	3	2.99	1.10		-5.8	-5.6	-7.6	0.0%	0.0%	0.0%
2,5-dianilinoterephthalic acid	233-302-8	10109-95-2	10109952	1314	Reach_2282	1718	3.05	0.65	3				-5.1	-5.6	-7.1	0.0%	0.0%	0.0%
6-[(p-tosyl)amino]hexanoic acid, compound with 2,2',2''-nitrilotri	301-097-5	93981-14-7	93981147	6086	Reach_3005	1719	5.58	0.79	3	4.58	0.79		-5.3	-5.6	-7.0	0.0%	0.0%	0.0%
diethyl maleate	600-786-0	106904-09-0	106904090	1448	Reach_4075	1720	5.00		1				-5.8	-5.6	-6.9	0.0%	0.0%	0.0%
tetramethyl 2,2'-[1,4-phenylenebis[imino(1-acetyl-2-oxoethane-	271-176-6	68516-73-4	68516734	3518	Reach_2907	1721	5.37	0.23	3	4.37	0.23		-5.1	-5.6	-7.2	0.0%	0.0%	0.0%
bis(2,4,4-trimethylpentyl)phosphinic acid	619-785-1	249561-98-6	249561986	5794	Reach_4545	1722							-5.4	-5.6	-6.9	0.0%	0.0%	0.0%
1-cyanoallyl acetate	201-855-4	88-74-4	88744	987	Reach_331	1723	4.63	0.70	28	3.63	0.70		-5.8	-5.6	-7.0	0.0%	0.0%	0.0%
608-497-1	611-000-0	5344-48-9	5344489	5922	Reach_4345	1724							-5.0	-5.6	-7.1	0.0%	0.0%	0.0%
606-097-1	606-097-1	186817-80-1	186817801	2203	Reach_4193	1725	4.76	0.59	3	3.76	0.59		-5.8	-5.6	-7.2	0.0%	0.0%	0.0%
2-phenoxyethyl isobutyrate	203-127-1	103-60-6	103606	1374	Reach_609	1726	4.16	0.29	3	3.48	0.53		-5.8	-5.6	-6.9	0.0%	0.0%	0.0%
diammonium 2,2'-dithiodiacetate	269-323-4	68223-93-8	68223938	5995	Reach_2901	1727	6.04	1.35	3	5.04	1.35		-5.4	-5.6	-7.0	0.0%	0.0%	0.0%
fluorobenzene	207-321-7	462-06-6	462066	643	Reach_1285	1728	3.93	0.15	3	2.93	0.15		-5.9	-5.6	-7.6	0.0%	0.0%	0.0%
2,2'-methylenediphenyl diisocyanate	219-799-4	2536-05-2	2536052	1249	Reach_1833	1729	6.37	0.26	3	5.37	0.26		-5.7	-5.6	-7.0	0.0%	0.0%	0.0%
N-(3-{[(dimethyl{3-[(2-methylacryloyl)amino]propyl}ammonio)ac	700-055-7	630113-05-2	630113052	5959	Reach_4743	1730	4.84	0.50	3	3.87	0.75		-5.3	-5.6	-7.0	0.0%	0.0%	0.0%
3-hydroxy-2'-methyl-2-naphthanilide	205-205-0	135-61-5	135615	1893	Reach_1132	1731	3.32		1				-5.0	-5.6	-7.1	0.0%	0.0%	0.0%
N,N,N',N',N'',N''-hexamethyl-1,3,5-triazine-1,3,5(2H,4H,6H)-tripr	240-004-1	15875-13-5	15875135	2064	Reach_2403	1732	4.84		2				-4.7	-5.6	-7.5	0.0%	0.0%	0.0%
cis-2,6-dimethylmorpholine	202-282-2	93-84-5	93845	4090	Reach_408	1733	4.70		1				-5.8	-5.6	-7.0	0.0%	0.0%	0.0%
benzophenone-3,3':4,4'-tetracarboxylic dianhydride	214-012-0	1072-63-5	1072635	1457	Reach_1642	1734	5.60	0.24	3	4.85	0.27		-5.0	-5.6	-7.1	0.0%	0.0%	0.0%
dimethyl maleate	210-848-5	624-48-6	624486	3369	Reach_1452	1735	3.95	0.38	3	2.95	0.38		-5.8	-5.6	-7.2	0.0%	0.0%	0.0%
2-ethylhexyl stearate	244-754-0	22047-49-0	22047490	2316	Reach_2515	1736	6.26	0.85	3	5.26	0.85		-5.8	-5.6	-6.2	0.0%	0.0%	0.0%
3-oxopregn-4-ene-21,17α-carbolactone	213-552-4	976-70-5	976705	4169	Reach_1622	1737	4.43		1				-5.0	-5.6	-7.1	0.0%	0.0%	0.0%
3-hydroxy-2,2-dimethylpropyl 3-hydroxy-2,2-dimethylpropionat	212-876-3	875-74-1	875741	3936	Reach_1583	1738	4.68	0.94	3				-4.9	-5.6	-7.2	0.0%	0.0%	0.0%
α,α,α-trifluoro-m-cresol	202-645-5	98-17-9	98179	1069	Reach_502	1739	4.01	0.84	16	3.01	0.84		-5.8	-5.6	-6.6	0.0%	0.0%	0.0%
601-332-4	603-436-5	13076-17-0	13076170	1843	Reach_4121	1740	5.75	0.50	3	5.14	0.48		-5.0	-5.6	-7.1	0.0%	0.0%	0.0%
1,1,1,3,3-pentachlorobutane	244-691-9	21981-33-9	21981339	2314	Reach_2512	1741	3.26		1				-5.9	-5.6	-7.7	0.0%	0.0%	0.0%
hex-3-yne-2,5-diol	206-687-5	367-25-9	367259	2774	Reach_1253	1742	3.70	0.47	3				-4.8	-5.6	-7.3	0.0%	0.0%	0.0%
ethyl chloroformate	208-778-5	541-41-3	541413	3129	Reach_1340	1743	4.94	1.87	4	3.94	1.87		-5.9	-5.6	-7.3	0.0%	0.0%	0.0%
1,2-diphenoxyethane	204-847-9	127-52-6	127526	1186	Reach_1099	1744	3.35	1.18	4	2.35	1.18		-5.8	-5.6	-7.0	0.0%	0.0%	0.0%
tridecane	211-093-4	629-50-5	629505	3389	Reach_1467	1745	5.93	2.45	3	4.93	2.45		-5.8	-5.6	-7.8	0.0%	0.0%	0.0%
panthenol , DL-form	240-540-6	16485-10-2	16485102	2094	Reach_2422	1746	5.23	1.64	3	5.00			-4.6	-5.6	-7.2	0.0%	0.0%	0.0%
amantadine	229-713-7	6674-22-2	6674222	3481	Reach_2201	1747	5.29	0.30	3	4.29	0.30		-5.8	-5.6	-6.9	0.0%	0.0%	0.0%
diallyl carbonate	219-340-8	2420-17-9	2420179	2377	Reach_1802	1748	3.56		2				-5.8	-5.6	-6.8	0.0%	0.0%	0.0%
chlorocresol	220-672-0	2857-97-8	2857978	2538	Reach_1877	1749	4.53	0.24	3				-5.8	-5.6	-6.5	0.0%	0.0%	0.0%
dibutyl phosphonate	217-316-1	1809-19-4	1809194	2164	Reach_1722	1750	5.23	0.91	3	4.10	0.83		-5.7	-5.6	-7.2	0.0%	0.0%	0.0%
Ammonium 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoa	700-242-3	62037-80-3	62037803	5953	Reach_4817	1751	4.85	0.53	3	3.85	0.53		-5.4	-5.6	-7.0	0.0%	0.0%	0.0%
L-valine	200-773-6	72-18-4	72184	3599	Reach_105	1752	5.01	1.04	3				-4.5	-5.6	-7.3	0.0%	0.0%	0.0%
2,4-dichloro-5-isopropoxyaniline	255-258-9	41200-96-8	41200968	2871	Reach_2739	1753	3.45	0.42	3				-5.2	-5.6	-7.3	0.0%	0.0%	0.0%
4-cyanophenyl acetate	235-893-8	13031-41-9	13031419	1835	Reach_2318	1754	4.13		1				-5.8	-5.6	-7.2	0.0%	0.0%	0.0%
oleonitrile	204-016-0	112-91-4	112914	1610	Reach_929	1755	1.48		1				-5.7	-5.6	-7.6	0.0%	0.0%	0.0%
tert-butyl (1R,3S,4S)-3-(5-bromo-1H-benzimidazol-2-yl)-2-azabic	700-743-7	161798-03-4	161798034	2082	Reach_4983	1756	2.78	0.29	3				-5.0	-5.6	-7.1	0.0%	0.0%	0.0%
valeraldehyde	203-784-4	110-62-3	110623	280	Reach_821	1757	4.41	0.37	4	3.41	0.37		-5.8	-5.6	-7.0	0.0%	0.0%	0.0%
613-982-6	249-020-3	28443-50-7	28443507	2530	Reach_2617	1758	3.20		1				-5.8	-5.6	-7.1	0.0%	0.0%	0.0%
diethyl peroxydicarbonate	238-707-3	14666-78-5	14666785	1992	Reach_2367	1759	4.35	0.71	3				-5.8	-5.6	-7.2	0.0%	0.0%	0.0%
trimethoxyphenylsilane	221-066-9	2996-92-1	2996921	2582	Reach_1894	1760	5.67	0.54	3	2.63	1.66		-5.8	-5.6	-6.8	0.0%	0.0%	0.0%
2-phenoxyethyl acrylate	256-360-6	48145-04-6	48145046	2972	Reach_2760	1761	3.60	0.41	3	2.60	0.41		-5.8	-5.6	-7.1	0.0%	0.0%	0.0%
N-(1,1,3,3-tetramethylbutyl)acrylamide	224-169-7	4223-03-4	4223034	1266	Reach_2021	1762	4.67	0.56	3	3.67	0.56		-5.8	-5.6	-7.2	0.0%	0.0%	0.0%
isobutyl methacrylate	202-613-0	97-86-9	97869	4174	Reach_489	1763	4.81	0.87	3	3.55	1.21		-5.9	-5.6	-7.2	0.0%	0.0%	0.0%
(1S,7S,8S,8aR)-8-{2-[(2R,4R)-4-hydroxy-6-oxotetrahydro-2H-pyra	691-746-1	220380-44-9	220380449	1241	Reach_4671	1764							-5.0	-5.6	-7.1	0.0%	0.0%	0.0%
N,N-dimethyldecan-1-amide	238-405-1	14433-76-2	14433762	471	Reach_2366	1765	4.03	0.26	5	3.00	0.19		-5.9	-5.6	-7.4	0.0%	0.0%	0.0%
609-118-2	600-451-9	103577-40-8	103577408	1371	Reach_4064	1766	2.82	0.21	3				-5.7	-5.6	-7.1	0.0%	0.0%	0.0%
5-hydroxyisophthalic acid	606-793-5	21535-43-3	21535433	2297	Reach_4218	1767	3.67		1				-4.9	-5.6	-7.2	0.0%	0.0%	0.0%
triacetoxyethylsilane	241-677-4	17689-77-9	17689779	2148	Reach_2441	1768	5.63	0.92	3	4.50	0.45		-5.8	-5.6	-7.2	0.0%	0.0%	0.0%
triethoxy(phenyl)silane	212-305-8	780-69-8	780698	891	Reach_1546	1769	5.01	0.67	5	3.68	0.79		-5.8	-5.6	-6.8	0.0%	0.0%	0.0%
glutamic acid	200-293-7	56-86-0	56860	3214	Reach_32	1770	5.24	0.43	3	4.24	0.43		-4.6	-5.6	-7.4	0.0%	0.0%	0.0%
tetrahydro-4-methylphthalic anhydride	251-823-9	34090-76-1	34090761	2690	Reach_2670	1771	5.00	0.17	3	4.33	0.23		-5.8	-5.6	-7.2	0.0%	0.0%	0.0%
pseudoephedrine	202-018-6	90-82-4	90824	4008	Reach_368	1772	5.13	0.55	3	4.06	0.49		-5.8	-5.6	-7.3	0.0%	0.0%	0.0%
triethyl orthoformate	204-550-4	122-51-0	122510	1750	Reach_1029	1773	5.47	0.42	3	4.08	0.61		-5.9	-5.6	-6.7	0.0%	0.0%	0.0%
(1S)-1-(3-methoxyphenyl)ethanamine	619-058-9	94695-48-4	94695484	4107	Reach_4509	1774	3.53	0.94	3				-5.8	-5.6	-7.1	0.0%	0.0%	0.0%
DL-malic acid	210-514-9	617-48-1	617481	3352	Reach_1435	1775	5.38		1				-4.6	-5.6	-7.3	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide	278-355-8	75980-60-8	75980608	3692	Reach_2946	1776	3.61	0.13	3	2.61	0.13		-5.6	-5.6	-7.1	0.0%	0.0%	0.0%
2-[(4-chloro-2-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxobuty	236-852-7	13515-40-7	13515407	1887	Reach_2340	1777	4.43	0.90	3	3.43	0.90		-5.1	-5.6	-7.0	0.0%	0.0%	0.0%
dimethyl 5-methylpyridine-2,3-dicarboxylate	214-625-3	1170-02-1	1170021	1654	Reach_1665	1778	4.15	0.58	3				-5.8	-5.7	-7.1	0.0%	0.0%	0.0%
N,N'-dithiodi-o-phenylenedibenzamide	205-201-9	135-57-9	135579	1891	Reach_1131	1779	1.98		1				-5.1	-5.7	-7.2	0.0%	0.0%	0.0%
6,6'-di-tert-butyl-4,4'-thiodi-m-cresol	202-525-2	96-69-5	96695	4152	Reach_469	1780	3.03	0.98	3	2.03	0.98		-5.3	-5.7	-6.3	0.0%	0.0%	0.0%
ethyl chloroacetate	203-294-0	105-39-5	105395	173	Reach_639	1781	3.47	0.44	4	2.47	0.44		-5.9	-5.7	-6.7	0.0%	0.0%	0.0%
2-(3,6-dihydroxy-2,4,5,7-tetrabromoxanthen-9-yl)-benzoic acid	604-351-6	143390-89-0	143390890	470	Pest_74	1782	2.20	0.46	11	2.07	0.57	8	-5.2	-5.7	-7.1	0.0%	0.0%	0.0%
N,N,N-trimethylanilinium chloride	260-126-9	56358-17-9	56358179	3192	Reach_2814	1783	3.28	1.64	3	2.28	1.64		-5.4	-5.7	-7.0	0.0%	0.0%	0.0%
pin-2(10)-ene	204-872-5	127-91-3	127913	412	Reach_1102	1784	2.90	0.70	8	1.90	0.70		-5.9	-5.7	-7.7	0.0%	0.0%	0.0%
N,N-dimethyldecylamine N-oxide	220-020-5	2605-79-0	2605790	2452	Reach_1844	1785	3.35	0.95	3	2.49	0.43		-5.3	-5.7	-7.2	0.0%	0.0%	0.0%
phenyl isocyanate	228-528-9	6289-46-9	6289469	3381	Reach_2161	1786	4.71		1				-5.9	-5.7	-6.9	0.0%	0.0%	0.0%
1-(1,3-benzodioxol-5-yl)propan-1-one	248-937-6	28281-49-4	28281494	2526	Reach_2616	1787							-5.8	-5.7	-7.2	0.0%	0.0%	0.0%
2,6-di-tert-butylphenol	204-884-0	128-39-2	128392	1820	Reach_1109	1788	3.27	0.52	3	2.50	0.61		-5.9	-5.7	-7.1	0.0%	0.0%	0.0%
3-(isodecyloxy)propiononitrile	613-099-6	62889-66-1	62889661	3379	Reach_4380	1789	3.00	1.04	3	2.02	0.87		-5.9	-5.7	-6.7	0.0%	0.0%	0.0%
604-018-5	604-018-5	137433-01-3	137433013	5682	Reach_4137	1790							-5.4	-5.7	-7.0	0.0%	0.0%	0.0%
[4-[α-[4-(dimethylamino)phenyl]benzylidene]cyclohexa-2,5-dien	255-288-2	41272-40-6	41272406	5879	Reach_2742	1791	3.19	0.66	3	2.19	0.66		-5.4	-5.7	-7.0	0.0%	0.0%	0.0%
4'-aminoazobenzene-4-sulphonic acid	203-187-9	104-23-4	104234	1388	Reach_620	1792	4.56	0.33	3	3.56	0.33		-4.8	-5.7	-7.3	0.0%	0.0%	0.0%
3,3-Dimethoxy-8,8,9,9-tetramethyl-2-oxa-7-thia-3,8-disiladecane	700-413-2	6331-96-0	6331960	3399	Reach_4891	1793	5.46	0.13	3	4.46	0.13		-5.9	-5.7	-7.2	0.0%	0.0%	0.0%
diphenyl methylphosphonate	231-388-1	7526-26-3	7526263	3659	Reach_2257	1794	3.90	0.45	3	3.12	0.40		-5.9	-5.7	-7.1	0.0%	0.0%	0.0%
ethyl 3-ethoxypropionate	212-112-9	763-69-9	763699	3710	Reach_1537	1795	5.62	0.62	3	4.62	0.62		-5.9	-5.7	-7.1	0.0%	0.0%	0.0%
cyclododecanol	217-031-2	1724-39-6	1724396	2126	Reach_1713	1796	3.71	0.15	3	2.71	0.15		-5.8	-5.7	-7.1	0.0%	0.0%	0.0%
xylitol	201-788-0	87-99-0	87990	3944	Reach_315	1797	7.94	0.51	3	6.94	0.51		-4.9	-5.7	-7.4	0.0%	0.0%	0.0%
2-aminobutan-1-ol	202-488-2	96-20-8	96208	4141	Reach_454	1798	3.91		2				-5.6	-5.7	-7.3	0.0%	0.0%	0.0%
3-amino-2-hydroxy-5-nitrobenzenesulphonic acid	202-523-1	96-67-3	96673	4151	Reach_468	1799	5.51	0.97	3	4.51	0.97		-4.6	-5.7	-7.5	0.0%	0.0%	0.0%
2-chloro-6-nitrotoluene	700-290-5	63968-64-9	63968649	3421	Reach_4844	1800	3.85	1.12	3				-5.9	-5.7	-6.8	0.0%	0.0%	0.0%
diisodecyl maleate	258-806-5	53817-61-1	53817611	3111	Reach_2794	1801	1.52	1.48	3				-5.7	-5.7	-6.4	0.0%	0.0%	0.0%
isobutyl (S)-2-chloropropionate	280-349-5	83261-15-8	83261158	3844	Reach_2965	1802	4.72	0.36	3	3.67	0.26		-5.9	-5.7	-7.2	0.0%	0.0%	0.0%
ditetradecyl fumarate	233-739-4	10341-03-4	10341034	1364	Reach_2289	1803	-0.09	2.89	3				-5.9	-5.7	-5.6	0.0%	0.0%	0.0%
3-amino-4-hydroxy-5-nitrobenzenesulphonic acid	251-868-4	34184-82-2	34184822	2693	Reach_2672	1804	4.53	0.21	3				-4.6	-5.7	-7.5	0.0%	0.0%	0.0%
2,3-epoxypropyl methacrylate	203-441-9	106-91-2	106912	1449	Reach_681	1805	4.10	0.40	3	3.10	0.40		-5.9	-5.7	-7.2	0.0%	0.0%	0.0%
608-245-0	608-245-0	28770-01-6	28770016	2544	Reach_4267	1806	4.93		1				-5.1	-5.7	-7.3	0.0%	0.0%	0.0%
cyclohexanone oxime	209-378-3	574-93-6	574936	3230	Reach_1378	1807	5.40		2	3.00			-5.7	-5.7	-7.1	0.0%	0.0%	0.0%
3,3'-Diisopropyl-5,5',6,6'-tetramethylbiphenyl-2,2'-diol	202-772-6	99-61-6	99616	1090	Reach_533	1808	3.76		1				-5.4	-5.7	-6.2	0.0%	0.0%	0.0%
naphthalene-1,8-dicarboximide	610-979-1	53207-58-2	53207582	3091	Reach_4343	1809	4.15		1				-4.9	-5.7	-7.3	0.0%	0.0%	0.0%
2,2'-(octadec-9-enylimino)bisethanol	246-807-3	25307-17-9	25307179	2429	Reach_2565	1810	1.90	0.73	3	0.90	0.73		-5.3	-5.7	-6.7	0.0%	0.0%	0.0%
2,3-dihydroxypropyl laurate	205-526-6	142-18-7	142187	1949	Reach_1173	1811	5.47		1	4.00			-5.2	-5.7	-7.2	0.0%	0.0%	0.0%
610-950-3	611-813-0	5926-26-1	5926261	3271	Reach_4365	1812							-5.9	-5.7	-6.8	0.0%	0.0%	0.0%
2-[(4-chloro-2-nitrophenyl)azo]-N-(2-chlorophenyl)-3-oxobutyrar	229-355-1	6486-23-3	6486233	3446	Reach_2191	1813	4.43	0.90	3	3.43	0.90		-5.0	-5.7	-7.1	0.0%	0.0%	0.0%
dioctadecyl disulphide	219-702-5	2500-88-1	2500881	2411	Reach_1824	1814	5.58	0.25	3	4.58	0.25		-5.9	-5.7	-3.8	0.0%	0.0%	0.0%
N,N'-ethylenebis(3,4,5,6-tetrabromophthalimide)	251-118-6	32588-76-4	32588764	2656	Reach_2663	1815	1.17	0.58	3				-5.6	-5.7	-6.1	0.0%	0.0%	0.0%
2-nitro-p-toluidine	201-924-9	89-62-3	89623	991	Reach_347	1816	4.04	0.49	5	3.04	0.70		-5.9	-5.7	-6.5	0.0%	0.0%	0.0%
propyl chloroformate	210-438-6	615-60-1	615601	3339	Reach_1428	1817	3.34	0.16	3	2.32	0.15		-5.9	-5.7	-7.4	0.0%	0.0%	0.0%
trichloro(vinyl)silane	200-917-8	75-94-5	75945	3690	Reach_167	1818	5.44	0.19	3	4.44	0.19		-5.9	-5.7	-7.9	0.0%	0.0%	0.0%
Octan-2-yl cyanoacetate	298-791-2	93839-21-5	93839215	4088	Reach_3000	1819							-5.9	-5.7	-7.1	0.0%	0.0%	0.0%
guanidinium chloride	203-533-9	107-93-7	107937	225	Reach_720	1820	5.25	0.79	3	4.25	0.79		-5.8	-5.7	-7.2	0.0%	0.0%	0.0%
nitromethane	200-876-6	75-52-5	75525	860	Reach_148	1821	5.37	0.54	4	4.51	0.98		-5.9	-5.7	-6.7	0.0%	0.0%	0.0%
7,8-didehydrocholesterol	223-028-7	3698-89-3	3698893	2787	Reach_1983	1822	1.95		3				-5.4	-5.7	-6.2	0.0%	0.0%	0.0%
2-ethylhexyl diphenyl phosphate	214-987-2	1241-94-7	1241947	403	Reach_1675	1823	2.84	0.87	5	2.09	0.80		-5.8	-5.7	-6.7	0.0%	0.0%	0.0%
bis(2,3-epoxypropyl) terephthalate	230-565-0	7195-44-0	7195440	3595	Reach_2230	1824	4.04	0.80	3	2.53	0.39		-5.2	-5.7	-7.4	0.0%	0.0%	0.0%
5-vinylnorborn-2-ene	605-460-1	167004-78-6	167004786	2110	Reach_4176	1825	3.58	0.39	3	2.40	0.87		-5.9	-5.7	-7.7	0.0%	0.0%	0.0%
diallyl phthalate	205-016-3	131-17-9	131179	418	Reach_1120	1826	3.66	0.72	5	2.75	0.66		-5.9	-5.7	-7.1	0.0%	0.0%	0.0%
2'-chloroacetoacetanilide	202-269-1	93-70-9	93709	4080	Reach_407	1827	4.89	0.39	3	3.89	0.39		-5.0	-5.7	-7.4	0.0%	0.0%	0.0%
3-3-diphenylpropylamine	255-670-9	42125-46-2	42125462	2889	Reach_2749	1828	3.41	0.79	3	3.44	0.93		-5.9	-5.7	-7.1	0.0%	0.0%	0.0%
dibutylamine	203-921-8	111-92-2	111922	317	Reach_882	1829	4.44	0.70	28	3.36	0.70		-5.9	-5.7	-7.0	0.0%	0.0%	0.0%
2,2,2-trifluoroethanol	200-913-6	75-89-8	75898	866	Reach_165	1830	5.79	0.49	3	4.79	0.49		-5.9	-5.7	-6.8	0.0%	0.0%	0.0%
pentamethylenediamine	207-329-0	462-94-2	462942	2950	Reach_1286	1831	5.18	1.06	3	4.18	1.06		-5.8	-5.7	-7.3	0.0%	0.0%	0.0%
bis(4-fluorophenyl) ketone	206-466-3	345-92-6	345926	2710	Reach_1240	1832	3.61	0.48	3	3.11	0.92		-5.9	-5.7	-7.1	0.0%	0.0%	0.0%
decanenitrile	217-830-6	1975-78-6	1975786	2239	Reach_1741	1833	3.21	0.72	3	2.21	0.72		-5.9	-5.7	-6.8	0.0%	0.0%	0.0%
(R)-p-mentha-1,8-diene	227-813-5	5989-27-5	5989275	743	Reach_2147	1834	3.73	0.75	9	2.61	0.86		-5.9	-5.7	-7.9	0.0%	0.0%	0.0%
p-(2-methoxyethyl)phenol	260-354-9	56718-71-9	56718719	3211	Reach_2821	1835	5.10	0.62	3	4.10	0.62		-5.9	-5.7	-7.3	0.0%	0.0%	0.0%
4-diazo-3,4-dihydro-7-nitro-3-oxonaphthalene-1-sulphonic acid	205-583-7	143-08-8	143088	469	Reach_1189	1836	4.04	0.33	6	3.04	0.33		-4.7	-5.7	-7.5	0.0%	0.0%	0.0%
nonan-4-olide	203-219-1	104-61-0	104610	1395	Reach_624	1837	4.17	0.44	3	3.35	0.60		-5.9	-5.7	-7.1	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
p-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	225-716-2	5026-74-4	5026744	3000	Reach_2071	1838	4.05	0.34	3	3.05	0.34		-4.9	-5.7	-7.4	0.0%	0.0%	0.0%
2,2'-oxydi(ethylamine)	220-395-5	2752-17-2	2752172	2511	Reach_1863	1839	4.97	0.95	3	3.97	0.95		-5.7	-5.7	-7.4	0.0%	0.0%	0.0%
dibromomethane	200-824-2	74-95-3	74953	842	Reach_118	1840	4.87	0.22	3	4.40	0.96		-6.0	-5.7	-7.4	0.0%	0.0%	0.0%
Ethyl N-pyridin-2-yl-beta-alaninate	201-756-6	87-60-5	87605	3937	Reach_312	1841	3.95		2				-5.6	-5.7	-7.3	0.0%	0.0%	0.0%
3-acetoxymethylen-7-amino-8-oxo-5-thia-1-azabicyclo[4.2.0]oct	213-485-0	957-68-6	957686	4133	Reach_1617	1842	5.39		2				-4.6	-5.7	-7.4	0.0%	0.0%	0.0%
N,N'-bis(1,3-dimethylbutylidene)-2,2'-iminobis(ethylamine)	234-205-3	10595-60-5	10595605	1423	Reach_2301	1843	5.35		2				-5.5	-5.7	-6.7	0.0%	0.0%	0.0%
607-449-7	607-449-7	24863-70-5	24863705	2405	Reach_4241	1844	4.32	0.27	3	3.32	0.24		-5.9	-5.7	-7.1	0.0%	0.0%	0.0%
diethyl malonate	203-305-9	105-53-3	105533	177	Reach_641	1845	5.02	0.69	4	4.02	0.75		-5.9	-5.7	-7.2	0.0%	0.0%	0.0%
4-chloro-N-cyclopentylbenzylamine	700-544-5	641571-10-0	641571100	3427	Reach_4930	1846	2.29	0.17	3				-5.9	-5.7	-6.9	0.0%	0.0%	0.0%
2-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]	250-830-4	31837-42-0	31837420	2639	Reach_2658	1847	4.17	1.01	3	3.17	1.01		-5.0	-5.7	-7.4	0.0%	0.0%	0.0%
dibenzylamine	203-117-7	103-49-1	103491	1368	Reach_607	1848	3.89	0.82	3	2.89	0.82		-5.9	-5.7	-7.0	0.0%	0.0%	0.0%
ethylene distearate	264-261-4	63469-23-8	63469238	3403	Reach_2859	1849	4.75		1				-5.9	-5.7	-4.8	0.0%	0.0%	0.0%
4'-methylacetophenone	204-514-8	122-00-9	122009	1740	Reach_1023	1850	4.50	0.23	3	3.50	0.23		-5.9	-5.7	-6.9	0.0%	0.0%	0.0%
heptane	205-563-8	142-82-5	142825	463	Reach_1180	1851	4.58	1.26	7	3.58	0.70		-6.0	-5.7	-8.2	0.0%	0.0%	0.0%
3-bromopropene	202-728-6	99-08-1	99081	1082	Reach_526	1852	4.36	0.70	28	3.11	0.38		-6.0	-5.7	-7.9	0.0%	0.0%	0.0%
1,2-epoxybutane	203-438-2	106-88-7	106887	1447	Reach_679	1853	5.26	0.32	3	4.26	0.32		-6.0	-5.7	-7.3	0.0%	0.0%	0.0%
610-840-5	226-006-5	5208-93-5	5208935	3052	Reach_2085	1854	3.62	0.41	3	2.62	0.46		-5.7	-5.7	-7.5	0.0%	0.0%	0.0%
617-500-5	205-187-4	135-37-5	135375	5673	Reach_1130	1855	5.36	0.33	3	4.13	0.80		-5.2	-5.7	-7.1	0.0%	0.0%	0.0%
3-chloro-p-tolyl isocyanate	611-435-6	56962-04-0	56962040	3217	Reach_4359	1856	3.44	0.36	3	2.44	0.36		-5.9	-5.7	-7.0	0.0%	0.0%	0.0%
600-261-6	604-776-7	151213-15-9	151213159	2018	Reach_4163	1857							-5.0	-5.7	-7.3	0.0%	0.0%	0.0%
2,2-bis[[(1-oxopentyl)oxy]methyl]propane-1,3-diyl divalerate	239-937-7	15834-04-5	15834045	2060	Reach_2402	1858	5.13	0.96	3	4.13	0.96		-5.4	-5.7	-6.8	0.0%	0.0%	0.0%
diethyl sulphate	200-589-6	64-67-5	64675	3442	Reach_73	1859	4.19	1.12	3				-5.9	-5.7	-7.2	0.0%	0.0%	0.0%
1-chlorobutane	203-696-6	109-69-3	109693	261	Reach_785	1860	5.88	0.59	3	4.86	0.57		-6.0	-5.7	-7.8	0.0%	0.0%	0.0%
eugenol	202-589-1	97-53-0	97530	1057	Reach_480	1861	3.99	0.54	4	3.15	0.53		-5.9	-5.7	-7.0	0.0%	0.0%	0.0%
2,4-difluoroaniline	242-615-9	18835-33-1	18835331	2210	Reach_2469	1862	6.38	0.27	3	5.38	0.27		-5.3	-5.7	-7.3	0.0%	0.0%	0.0%
trimethoxy(methyl)silane	214-685-0	1185-55-3	1185553	1672	Reach_1666	1863	5.51	0.67	3	4.51	0.67		-6.0	-5.7	-7.2	0.0%	0.0%	0.0%
(S)-(+)-2-(2-Chlorophenyl)-2-hydroxyacetic acid	700-307-6	52950-19-3	52950193	5918	Reach_4853	1864							-5.5	-5.7	-7.1	0.0%	0.0%	0.0%
(2E)-3,7-dimethylocta-2,6-dien-1-amine	624-182-1	4187-38-6	4187386	2885	Reach_4579	1865	4.30		2				-5.9	-5.7	-7.2	0.0%	0.0%	0.0%
N-[4-(aminocarbonyl)phenyl]-4-nitrobenzamide	610-886-6	52688-08-1	52688081	3068	Reach_4338	1866	3.64	0.65	3				-4.9	-5.7	-7.5	0.0%	0.0%	0.0%
3,9-bis(2,4-di-tert-butylphenoxy)-2,4,8,10-tetraoxa-3,9-diphosph	247-952-5	26741-53-7	26741537	2485	Reach_2591	1867	4.37	0.90	3	3.37	0.90		-5.8	-5.7	-6.1	0.0%	0.0%	0.0%
4,5-dihydroxy-1,3-dimethylimidazolidin-2-one	223-496-2	3923-79-3	3923793	2836	Reach_2002	1868	4.95	2.71	3				-4.7	-5.7	-7.5	0.0%	0.0%	0.0%
1,3,5-triallyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	606-251-8	1917-44-8	1917448	2224	Reach_4201	1869	3.64		1				-5.2	-5.7	-7.1	0.0%	0.0%	0.0%
5-(4-hydroxyphenyl)imidazolidine-2,4-dione	239-106-9	15022-08-9	15022089	2008	Reach_2375	1870	3.00		1				-4.9	-5.7	-7.3	0.0%	0.0%	0.0%
N-lauroylsarcosine	202-608-3	97-78-9	97789	4172	Reach_488	1871	4.75	0.26	3	3.70	0.46		-5.3	-5.7	-7.3	0.0%	0.0%	0.0%
3-cyclopentyl-1H-indole-6-carboxylic acid	936-788-6	1307233-94-8	1307233948	1841	Reach_5143	1872							-5.2	-5.7	-7.3	0.0%	0.0%	0.0%
608-748-5	205-138-7	134-32-7	134327	430	Reach_1127	1873	4.39		2				-5.3	-5.7	-6.8	0.0%	0.0%	0.0%
2,4-dichloro-1,3-dinitro-5-(trifluoromethyl)benzene	249-420-8	29091-09-6	29091096	2557	Reach_2627	1874	2.30		1				-5.9	-5.7	-7.3	0.0%	0.0%	0.0%
phthaloyl dichloride	201-660-4	86-28-2	86282	3903	Reach_301	1875	3.50		1				-5.9	-5.7	-7.3	0.0%	0.0%	0.0%
isooctadecyl palmitate	614-477-3	6842-62-2	6842622	3515	Reach_4398	1876	2.03	0.56	3	1.03	0.56		-5.9	-5.7	-5.0	0.0%	0.0%	0.0%
isodecyl diphenyl phosphate	249-828-6	29761-21-5	29761215	588	Reach_2630	1877	5.04	1.19	5	4.04	1.19		-5.2	-5.7	-6.3	0.0%	0.0%	0.0%
6-amino-5-formamido-1,3-dimethyluracil	208-793-7	541-85-5	541855	686	Reach_1342	1878	4.88	0.41	4	3.88	0.41		-4.7	-5.7	-7.4	0.0%	0.0%	0.0%
1,3-dichloro-5-isocyanatobenzene	690-920-4	494799-38-1	494799381	2982	Reach_4662	1879	3.03	0.81	3				-6.0	-5.7	-6.9	0.0%	0.0%	0.0%
4-chloro-α,α,α-trifluorotoluene	202-681-1	98-56-6	98566	4187	Reach_513	1880	3.53	0.39	3	2.53	0.39		-6.0	-5.7	-7.9	0.0%	0.0%	0.0%
2-amino-4-nitrophenol	202-767-9	99-57-0	99570	4206	Reach_531	1881	4.83	0.39	3	3.83	0.39		-4.9	-5.7	-7.5	0.0%	0.0%	0.0%
O,O,O-triphenyl phosphorothioate	209-909-9	597-82-0	597820	3288	Reach_1401	1882	4.80		2				-5.6	-5.7	-6.8	0.0%	0.0%	0.0%
4-[(6-amino-1-hydroxy-3-sulpho-2-naphthyl)azo]-3-hydroxy-7-nit	700-424-2	6872-10-2	6872102	1286	Reach_4897	1883							-5.0	-5.7	-7.3	0.0%	0.0%	0.0%
(6R-trans)-7-amino-8-oxo-3-[[(1,2,5,6-tetrahydro-2-methyl-5,6-d	212-338-8	791-28-6	791286	95	Reach_1547	1884	4.63	0.23	4	3.72	0.32		-4.8	-5.7	-7.3	0.0%	0.0%	0.0%
607-301-1	700-490-2	36635-56-0	36635560	2772	Reach_4911	1885	5.19	0.53	3	4.19	0.53		-5.0	-5.7	-7.3	0.0%	0.0%	0.0%
2'-[2,4-dichloro-5-(1-methylethoxy)phenyl]-2,2-dimethylpropion	257-027-8	51167-18-1	51167181	3028	Reach_2769	1886	4.00	0.87	3	3.17	0.58		-5.6	-5.7	-7.2	0.0%	0.0%	0.0%
thiodiglycol	229-662-0	6642-31-5	6642315	3474	Reach_2200	1887							-5.0	-5.7	-7.4	0.0%	0.0%	0.0%
608-356-4	613-147-6	63141-09-3	63141093	3395	Reach_4382	1888	4.68		1				-5.9	-5.7	-6.8	0.0%	0.0%	0.0%
(1R)-1-Phenylpropan-1-amine	264-133-8	63422-71-9	63422719	3400	Reach_2857	1889	4.61	1.33	3				-5.9	-5.7	-6.8	0.0%	0.0%	0.0%
2-dibutylaminoethanol	203-057-1	102-81-8	102818	1354	Reach_599	1890	4.74	0.63	3	3.69	0.54		-6.0	-5.7	-7.3	0.0%	0.0%	0.0%
623-635-0	256-283-8	46830-22-2	46830222	5893	Reach_2758	1891	4.66	0.56	3	3.66	0.56		-6.0	-5.7	-6.8	0.0%	0.0%	0.0%
(1R)-1-(4-methylphenyl)ethanamine	632-902-0	82796-69-8	82796698	3837	Reach_4599	1892	4.72		1				-6.0	-5.7	-6.8	0.0%	0.0%	0.0%
N-(3-aminopropyl)-N-dodecylpropane-1,3-diamine	219-145-8	2372-82-9	2372829	554	Reach_1788	1893	2.27	0.84	6	1.43	0.69		-5.3	-5.7	-7.1	0.0%	0.0%	0.0%
salicylaldehyde	201-961-0	90-02-8	90028	998	Reach_356	1894	3.76	0.38	26	2.76	0.38	26	-6.0	-5.7	-7.2	0.0%	0.0%	0.0%
(2R)-3-cyano-2-hydroxy-N,N,N-trimethylpropan-1-aminium chlor	700-244-4	5895-82-9	5895829	3263	Reach_4819	1895							-5.5	-5.7	-7.1	0.0%	0.0%	0.0%
4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl	218-760-9	2226-96-2	2226962	2327	Reach_1775	1896	5.48	0.49	3	4.30	0.43		-4.9	-5.7	-7.4	0.0%	0.0%	0.0%
3-hydroxy-2-(hydroxymethyl)-2-methylpropionaldehyde	242-393-3	18516-18-2	18516182	2194	Reach_2464	1897	5.14		2				-5.0	-5.7	-7.4	0.0%	0.0%	0.0%
tert-butyl acrylate	216-768-7	1663-39-4	1663394	2103	Reach_1706	1898	3.72	0.52	3	2.86	0.52		-6.0	-5.7	-7.4	0.0%	0.0%	0.0%
4-amino-2-methylpyrimidine-5-methylamine	222-483-9	3490-06-0	3490060	2718	Reach_1968	1899	3.89	0.75	3				-5.0	-5.7	-7.3	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
l-p-mentha-1(6),8-dien-2-one	219-348-1	2421-28-5	2421285	2378	Reach_1803	1900	5.46	0.87	3	4.46	0.87		-6.0	-5.7	-6.8	0.0%	0.0%	0.0%
(2S,3S,3aR,9aS)-3-hydroxy-2-(hydroxymethyl)-7-methyl-	619-693-1	159276-62-7	159276627	2067	Reach_4537	1901	3.50	0.53	3				-4.8	-5.7	-7.5	0.0%	0.0%	0.0%
citronellal	203-376-6	106-23-0	106230	1432	Reach_660	1902	4.09	0.23	3	3.12	0.37		-6.0	-5.7	-7.0	0.0%	0.0%	0.0%
anisole	202-876-1	100-66-3	100663	136	Reach_567	1903	4.27	0.56	5	3.27	0.75		-6.0	-5.7	-6.9	0.0%	0.0%	0.0%
4-hydroxybenzenesulphonic acid	202-691-6	98-67-9	98679	4190	Reach_516	1904	5.62		2				-4.7	-5.7	-7.3	0.0%	0.0%	0.0%
4,11-dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione	696-317-2	174489-76-0	174489760	2138	Reach_4713	1905	3.01	0.41	3	2.01	0.41		-5.5	-5.8	-7.1	0.0%	0.0%	0.0%
dimethyl adipate	211-020-6	627-93-0	627930	3378	Reach_1460	1906	5.06		1				-5.9	-5.8	-7.2	0.0%	0.0%	0.0%
retinyl palmitate	201-228-5	79-81-2	79812	3784	Reach_250	1907	5.34	1.68	3	4.34	1.68		-6.0	-5.8	-5.1	0.0%	0.0%	0.0%
ethyldimethylamine	209-940-8	598-56-1	598561	741	Reach_1404	1908	4.54	0.66	4	3.53	0.70		-6.0	-5.8	-7.2	0.0%	0.0%	0.0%
606-964-4	201-153-8	78-88-6	78886	903	Reach_214	1909	4.99		1	4.60			-5.2	-5.8	-7.3	0.0%	0.0%	0.0%
3,7,7-trimethylbicyclo[4.1.0]hept-3-ene	236-719-3	13466-78-9	13466789	434	Reach_2337	1910	4.59		2				-6.0	-5.8	-7.8	0.0%	0.0%	0.0%
disodium 4,4'-bis[[6-anilino-4-[(2-hydroxyethyl)methylamino]-1,:	237-600-9	13863-31-5	13863315	1191	Reach_2350	1911	5.12	0.36	3	4.12	0.36		-5.5	-5.8	-7.1	0.0%	0.0%	0.0%
3,3'-(ethylenediimino)bispropiononitrile	607-936-4	26447-85-8	26447858	2469	Reach_4254	1912	4.71	0.95	3				-4.9	-5.8	-7.5	0.0%	0.0%	0.0%
potassium dimethyldithiocarbamate	204-875-1	128-03-0	128030	1187	Reach_1104	1913	2.30	0.67	7	1.50	0.54		-5.5	-5.8	-7.1	0.0%	0.0%	0.0%
2-ethyl-N,N-bis(2-ethylhexyl)hexylamine	278-575-4	76918-62-2	76918622	6033	Reach_2948	1914							-5.8	-5.8	-6.7	0.0%	0.0%	0.0%
isovaleric acid	207-975-3	503-74-2	503742	657	Reach_1302	1915	4.98	0.66	4	4.14	0.52		-5.7	-5.8	-7.2	0.0%	0.0%	0.0%
2-cyano-2-[2,3-dihydro-3-(tetrahydro-2,4,6-trioxo-5(2H)-pyrimid	278-388-8	76199-85-4	76199854	3703	Reach_2947	1916							-4.7	-5.8	-7.5	0.0%	0.0%	0.0%
1,3-dioxepane	208-015-6	505-65-7	505657	3010	Reach_1309	1917	5.33	1.45	3	4.33	1.45		-6.0	-5.8	-6.8	0.0%	0.0%	0.0%
(trimethoxysilyl)methyl prop-2-enoate	618-109-2	88069-93-6	88069936	3946	Reach_4486	1918	3.60	0.38	3				-5.2	-5.8	-7.5	0.0%	0.0%	0.0%
didodecyl fumarate	219-280-2	2402-58-6	2402586	2365	Reach_1794	1919	5.66		2				-5.9	-5.8	-6.2	0.0%	0.0%	0.0%
610-122-1	696-441-7	256473-05-9	256473059	2442	Reach_4717	1920	3.59	0.13	3	2.59	0.13		-4.9	-5.8	-7.5	0.0%	0.0%	0.0%
ursodeoxycholic acid	204-879-3	128-13-2	128132	1816	Reach_1107	1921	5.37	0.22	3	4.37	0.22		-5.2	-5.8	-7.3	0.0%	0.0%	0.0%
pentasodium bis[5-[(4-amino-6-chloro-1,3,5-triazin-2-yl)amino]-4	279-317-3	79828-43-6	79828436	6041	Reach_2957	1922	4.94		1				-5.5	-5.8	-7.1	0.0%	0.0%	0.0%
1,3-bis(1-isocyanato-1-methylethyl)benzene	220-474-4	2778-42-9	2778429	2517	Reach_1865	1923	3.39	0.48	3	2.38	0.33		-5.9	-5.8	-7.2	0.0%	0.0%	0.0%
diethyl ether	200-467-2	60-29-7	60297	750	Reach_57	1924	6.24	0.62	7	5.24	0.70		-6.0	-5.8	-7.4	0.0%	0.0%	0.0%
2'-anilino-6'-[ethyl(3-methylbutyl)amino]-3'-methylspiro[isobenz	274-641-1	70516-41-5	70516415	3563	Reach_2918	1925	5.30	0.96	3	4.30	0.96		-5.0	-5.8	-7.2	0.0%	0.0%	0.0%
604-351-6	603-567-8	132335-47-8	132335478	5666	Reach_4126	1926							-5.6	-5.8	-7.0	0.0%	0.0%	0.0%
furfurylamine	805-957-5	848655-78-7	848655787	3879	Reach_5071	1927	4.08	0.82	3				-6.0	-5.8	-7.1	0.0%	0.0%	0.0%
propane-1,3-diol	207-997-3	504-63-2	504632	660	Reach_1306	1928	6.67	0.30	4	5.67	0.30		-5.1	-5.8	-7.4	0.0%	0.0%	0.0%
3-(methylamino)propane-1,2-diol	254-809-0	40137-22-2	40137222	2853	Reach_2729	1929	5.06	1.06	3				-5.2	-5.8	-7.4	0.0%	0.0%	0.0%
2,9-bis(2-phenylethyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoquinolin	266-564-7	67075-37-0	67075370	3484	Reach_2884	1930	5.13	2.03	3	4.13	2.03		-5.6	-5.8	-7.1	0.0%	0.0%	0.0%
3',4'-dichloro-5-fluorobiphenyl-2-amine	203-360-9	106-09-2	106092	1427	Reach_655	1931	3.18	0.71	3				-5.3	-5.8	-7.3	0.0%	0.0%	0.0%
609-920-2	243-473-0	20030-30-2	20030302	2248	Reach_2487	1932	5.08	0.21	3	4.19	0.20		-5.0	-5.8	-7.3	0.0%	0.0%	0.0%
perhydroazepine	203-875-9	111-49-9	111499	304	Reach_860	1933	4.97	0.70	12	4.06	0.70		-6.0	-5.8	-6.7	0.0%	0.0%	0.0%
3,5-dichlorobenzoyl chloride	220-813-6	2905-62-6	2905626	2556	Reach_1882	1934	3.53	0.12	3				-6.0	-5.8	-7.0	0.0%	0.0%	0.0%
2-amino-5-nitrophenol	204-515-3	122-01-0	122010	1741	Reach_1024	1935	5.02	0.36	3	4.11	0.33		-4.9	-5.8	-7.5	0.0%	0.0%	0.0%
3-aminopropane-1,2-diol	210-475-8	616-30-8	616308	3343	Reach_1430	1936	4.90		2				-5.2	-5.8	-7.4	0.0%	0.0%	0.0%
dimethyl 2-aminoterephthalate	226-364-2	5372-81-6	5372816	683	Reach_2103	1937	4.01	0.08	3	3.03	0.12		-5.2	-5.8	-7.4	0.0%	0.0%	0.0%
triisotridecyl benzene-1,2,4-tricarboxylate	276-594-2	72361-35-4	72361354	3603	Reach_2936	1938	4.27	0.33	3	3.27	0.33		-6.0	-5.8	-3.8	0.0%	0.0%	0.0%
isodecyl diphenyl phosphite	247-777-4	26544-23-0	26544230	2476	Reach_2587	1939	1.41	0.36	3				-5.4	-5.8	-6.3	0.0%	0.0%	0.0%
2-ethylhexanoyl chloride	212-081-1	760-67-8	760678	3697	Reach_1531	1940	3.96	0.92	3	2.96	0.92		-6.0	-5.8	-7.6	0.0%	0.0%	0.0%
Methyl 3-[(2,2-dimethylbutanoyl)thio]propanoate	620-518-6	938063-63-9	938063639	4084	Reach_4574	1941	4.02	0.77	3				-6.0	-5.8	-7.3	0.0%	0.0%	0.0%
619-529-9	210-787-4	623-33-6	623336	5956	Reach_1448	1942							-5.1	-5.8	-7.3	0.0%	0.0%	0.0%
1,6,7,8,9,14,15,16,17,17,18,18-dodecachloropentacyclo[12.2.1.1	236-948-9	13560-89-9	13560899	1892	Reach_2341	1943	-0.43	0.97	3				-6.0	-5.8	-6.1	0.0%	0.0%	0.0%
3-diethylaminophenol	202-090-9	91-68-9	91689	4019	Reach_379	1944	4.32	0.34	3	3.07	0.10		-5.1	-5.8	-7.5	0.0%	0.0%	0.0%
acetone oxime	204-820-1	127-06-0	127060	410	Reach_1095	1945	5.39	0.65	4	4.39	0.65		-6.0	-5.8	-7.0	0.0%	0.0%	0.0%
N-(3-(trimethoxysilyl)propyl)ethylenediamine	217-164-6	1760-24-3	1760243	2145	Reach_1718	1946	5.06	0.76	3	4.24	0.72		-5.2	-5.8	-7.5	0.0%	0.0%	0.0%
1-amino-1-deoxy-D-glucitol	227-577-3	5894-79-1	5894791	3261	Reach_2143	1947	4.65	0.21	3				-4.9	-5.8	-7.5	0.0%	0.0%	0.0%
4-chlorobenzoyl chloride	619-326-5	98210-99-2	98210992	4180	Reach_4513	1948							-6.0	-5.8	-6.9	0.0%	0.0%	0.0%
chenodeoxycholic acid	207-481-8	474-25-9	474259	2966	Reach_1289	1949	5.37	0.22	3	4.37	0.22		-5.2	-5.8	-7.3	0.0%	0.0%	0.0%
N-(hydroxymethyl)methacrylamide	213-086-1	923-02-4	923024	4030	Reach_1592	1950	5.84	0.52	3	4.84	0.52		-4.8	-5.8	-7.4	0.0%	0.0%	0.0%
taurine	608-544-6	3082-64-2	3082642	2613	Reach_4277	1951	3.82	0.70	3				-4.9	-5.8	-7.5	0.0%	0.0%	0.0%
615-497-5	249-070-6	28535-81-1	28535811	2535	Reach_2620	1952	5.37	0.22	3	4.37	0.22		-5.5	-5.8	-7.1	0.0%	0.0%	0.0%
propyl 4-hydroxybenzoate	202-307-7	94-13-3	94133	109	Reach_412	1953	4.03	0.19	3	3.03	0.19		-5.9	-5.8	-7.3	0.0%	0.0%	0.0%
ethyl 2-cyanoacrylate	230-391-5	7085-85-0	7085850	3571	Reach_2224	1954	2.87	1.70	3				-6.0	-5.8	-7.2	0.0%	0.0%	0.0%
2-(2-naphthyloxy)ethanol	202-228-8	93-20-9	93209	4065	Reach_401	1955	4.28	0.24	3	3.37	0.43		-5.1	-5.8	-7.4	0.0%	0.0%	0.0%
methyl vinyl ether	203-475-4	107-25-5	107255	1456	Reach_702	1956	4.63	0.12	3	3.80	0.23		-6.1	-5.8	-7.6	0.0%	0.0%	0.0%
6-tert-butyl-m-cresol	201-842-3	88-60-8	88608	3961	Reach_327	1957	3.46	0.21	3	2.46	0.21		-6.0	-5.8	-7.3	0.0%	0.0%	0.0%
N,N'-bis(1,4-dimethylpentyl)-p-phenylenediamine	221-375-9	3081-14-9	3081149	2612	Reach_1913	1958	3.44	1.45	3	2.44	1.45		-5.9	-5.8	-7.1	0.0%	0.0%	0.0%
propane-1,2,3-triyl 3,5,5-trimethylhexanoate	260-257-1	56554-53-1	56554531	3202	Reach_2817	1959	1.08	0.74	3				-5.8	-5.8	-6.4	0.0%	0.0%	0.0%
ethanethiol	200-837-3	75-08-1	75081	849	Reach_128	1960	3.05	0.93	4	2.05	0.93		-6.0	-5.8	-7.7	0.0%	0.0%	0.0%
1-benzyl-1,2-dihydro-3H-indazol-3-one, sodium salt	236-138-5	13185-09-6	13185096	5663	Reach_2325	1961	4.62		1				-5.5	-5.8	-7.1	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
1-[4-(trans-4-propylcyclohexyl)phenyl]pentan-1-one	601-770-6	121315-20-6	121315206	1725	Reach_4103	1962	5.68		1				-5.5	-5.8	-6.6	0.0%	0.0%	0.0%
3,4-dichlorotoluene	700-475-0	145783-14-8	145783148	1988	Reach_4907	1963	1.69	0.36	3	0.66	0.24		-6.0	-5.8	-7.4	0.0%	0.0%	0.0%
2-methylbutan-2-ol	252-173-9	34730-59-1	34730591	5853	Reach_2682	1964							-6.0	-5.8	-6.8	0.0%	0.0%	0.0%
p-phenylbenzonitrile	220-860-2	2920-38-9	2920389	2561	Reach_1885	1965	3.86	0.12	3	2.86	0.12		-6.0	-5.8	-7.2	0.0%	0.0%	0.0%
trometamol	201-064-4	77-86-1	77861	3739	Reach_187	1966	6.34	0.90	3	5.34	0.90		-4.9	-5.8	-7.5	0.0%	0.0%	0.0%
2,9-bis(p-methoxybenzyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoquin	280-472-4	83524-75-8	83524758	3848	Reach_2967	1967	5.13	2.03	3	4.13	2.03		-5.7	-5.8	-7.1	0.0%	0.0%	0.0%
(Z)-N-9-octadecenylpropane-1,3-diamine	230-528-9	7173-62-8	7173628	3589	Reach_2229	1968	2.03	0.50	3	1.03	0.50		-5.8	-5.8	-7.2	0.0%	0.0%	0.0%
fluorene	201-695-5	86-73-7	86737	973	Reach_302	1969	3.38	0.78	11	2.38	0.70	44	-6.0	-5.8	-6.8	0.0%	0.0%	0.0%
dimethoxymethane	203-714-2	109-87-5	109875	268	Reach_795	1970	6.33	0.70	12	5.33	0.28		-6.1	-5.8	-7.2	0.0%	0.0%	0.0%
N-[4-(1,1,1,2,3,3,3-heptafluoropropan-2-yl)-2-methylphenyl]-N'-(	609-338-9	371771-07-2	371771072	2793	Reach_4299	1971	3.82		2				-5.2	-5.8	-7.1	0.0%	0.0%	0.0%
606-050-5	212-161-6	766-09-6	766096	874	Reach_1542	1972	4.56	0.70	12	3.56	0.70		-5.3	-5.8	-7.0	0.0%	0.0%	0.0%
12H-phthaloperin-12-one	202-549-3	96-98-0	96980	4159	Reach_474	1973	5.05		1				-5.1	-5.8	-7.3	0.0%	0.0%	0.0%
3-methylpyrazole	215-925-7	1453-58-3	1453583	1985	Reach_1683	1974	5.52	0.36	3	4.52	0.36		-4.9	-5.8	-7.3	0.0%	0.0%	0.0%
bis[2-[2-(1-methylethyl)-3-oxazolidinyl]ethyl] hexan-1,2-diylbisca	261-879-6	59719-67-4	59719674	3284	Reach_2841	1975	4.13	1.46	3	3.13	1.46		-5.2	-5.8	-7.4	0.0%	0.0%	0.0%
2-[[(4-methoxyphenyl)methylhydrazono]methyl]-1,3,3-trimethyl	261-448-2	58798-47-3	58798473	5941	Reach_2832	1976	3.26	1.14	3	2.27	1.44		-5.5	-5.8	-7.2	0.0%	0.0%	0.0%
arginine	200-811-1	74-79-3	74793	3644	Reach_107	1977	6.35		2				-4.7	-5.8	-7.5	0.0%	0.0%	0.0%
propane-1,2-diyl diacetate	210-817-6	623-84-7	623847	3367	Reach_1450	1978	5.19	0.27	3	4.19	0.27		-6.0	-5.8	-7.3	0.0%	0.0%	0.0%
620-464-3	700-287-9	877179-04-9	877179049	3939	Reach_4842	1979	2.60		1				-5.2	-5.8	-7.4	0.0%	0.0%	0.0%
2-amino-4-chloro-6-nitrophenol	234-234-1	10605-40-0	10605400	1426	Reach_2302	1980	4.09	0.16	3				-5.1	-5.8	-7.5	0.0%	0.0%	0.0%
1-bromopropane	203-445-0	106-94-5	106945	203	Reach_684	1981	4.73	0.70	16	3.26	0.70		-6.1	-5.8	-7.8	0.0%	0.0%	0.0%
stearoyl chloride	700-093-4	176969-34-9	176969349	2150	Reach_4758	1982	5.42	0.32	3	4.42	0.32		-5.9	-5.8	-7.9	0.0%	0.0%	0.0%
2,2'-methylenebis(6-nonyl-p-cresol)	232-092-5	7786-17-6	7786176	3740	Reach_2275	1983	-0.35	2.22	3				-6.0	-5.8	-6.0	0.0%	0.0%	0.0%
5-phenyl-o-anisidine	927-913-5	160844-75-7	160844757	2077	Reach_5115	1984	2.83	0.34	3				-5.4	-5.8	-7.3	0.0%	0.0%	0.0%
trifluoroacetic acid	200-929-3	76-05-1	76051	3695	Reach_171	1985	5.51	1.29	3	4.71	1.57		-5.0	-5.8	-7.4	0.0%	0.0%	0.0%
methyl octanoate	203-835-0	111-11-5	111115	1538	Reach_844	1986	4.38	1.03	3	3.38	1.03		-6.0	-5.8	-7.4	0.0%	0.0%	0.0%
di-sec-butylphenol	250-184-3	30414-53-0	30414530	2595	Reach_2645	1987	4.68	1.07	3				-5.9	-5.8	-7.2	0.0%	0.0%	0.0%
docosyl acrylate	242-182-6	18299-85-9	18299859	2177	Reach_2458	1988	-0.76	2.28	3	5.00			-6.0	-5.8	-6.6	0.0%	0.0%	0.0%
1,1'-(p-tolylimino)dipropan-2-ol	254-075-1	38668-48-3	38668483	2825	Reach_2717	1989	4.69	0.61	3	3.69	0.61		-5.2	-5.8	-7.5	0.0%	0.0%	0.0%
604-776-7	209-010-1	552-37-4	552374	5930	Reach_1359	1990							-5.0	-5.8	-7.3	0.0%	0.0%	0.0%
α,α,α-trifluoro-p-toluidine	207-236-5	455-14-1	455141	2941	Reach_1279	1991	3.67		2	2.66			-5.1	-5.8	-7.4	0.0%	0.0%	0.0%
1,3-dihydroxyacetone	202-494-5	96-26-4	96264	4143	Reach_458	1992	5.00		1				-5.2	-5.8	-7.5	0.0%	0.0%	0.0%
7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-3,6,8,1	253-211-7	36788-39-3	36788393	2777	Reach_2705	1993	5.93	1.15	3				-4.9	-5.8	-7.6	0.0%	0.0%	0.0%
5-[[4-chloro-6-[(3-sulphophenyl)amino]-1,3,5-triazin-2-yl]amino]	279-015-1	78952-61-1	78952611	6040	Reach_2955	1994	6.30		1				-5.6	-5.8	-7.2	0.0%	0.0%	0.0%
4-amino-2-methylpyrimidine-5-carbonitrile	609-474-9	37750-29-1	37750291	2805	Reach_4302	1995	3.26	0.55	3				-5.0	-5.8	-7.3	0.0%	0.0%	0.0%
butyl glycollate	223-664-5	4009-98-7	4009987	5874	Reach_2005	1996	3.34		1				-6.0	-5.8	-7.5	0.0%	0.0%	0.0%
N,N'-(2-chloro-1,4-phenylene)bis[4-[(4-chloro-2-nitrophenyl)azo]	217-589-7	1897-52-5	1897525	2217	Reach_1733	1997	5.05		1				-6.0	-5.8	-4.9	0.0%	0.0%	0.0%
α,α'-propylenedinitrilodi-o-cresol	202-374-2	94-91-7	94917	4116	Reach_419	1998	3.93	0.60	3	2.97	0.73		-5.1	-5.8	-7.5	0.0%	0.0%	0.0%
cis-propenylphosphonic acid	605-830-2	178671-69-7	178671697	2156	Reach_4182	1999							-5.0	-5.8	-7.3	0.0%	0.0%	0.0%
tetrabutylurea	224-929-8	4559-86-8	4559868	2943	Reach_2048	2000	3.12	0.20	3	2.12	0.20		-5.9	-5.8	-7.0	0.0%	0.0%	0.0%
609-474-9	700-807-4	134283-49-1	134283491	1877	Reach_4999	2001	3.52	0.50	3				-5.5	-5.8	-7.4	0.0%	0.0%	0.0%
octylamine	203-916-0	111-86-4	111864	313	Reach_877	2002	3.35	0.96	6	2.10	0.70		-6.1	-5.8	-7.3	0.0%	0.0%	0.0%
8-chloro-5,10-dihydro-11H-dibenzo[b,e][1,4]diazepin-11-one	203-242-7	104-83-6	104836	1401	Reach_630	2003	3.37		1				-5.3	-5.8	-7.5	0.0%	0.0%	0.0%
trimethylenediamine	202-288-5	93-92-5	93925	4093	Reach_409	2004	4.47	0.46	3	3.70	0.41		-6.0	-5.8	-7.2	0.0%	0.0%	0.0%
2-hexyldecan-1-ol	219-370-1	2425-77-6	2425776	2381	Reach_1805	2005	4.09	1.73	3	1.76	1.24		-5.9	-5.8	-7.0	0.0%	0.0%	0.0%
isometheptene	257-484-3	51867-77-7	51867777	3047	Reach_2775	2006	2.71	1.02	3				-6.0	-5.8	-6.9	0.0%	0.0%	0.0%
616-378-0	606-356-9	19708-81-7	19708817	2237	Reach_4205	2007	4.11	0.88	3				-5.3	-5.8	-7.5	0.0%	0.0%	0.0%
N,N,N',N'-tetramethylhexamethylenediamine	252-772-5	35869-64-8	35869648	2752	Reach_2695	2008	-0.61	3.44	3	4.00			-6.0	-5.8	-7.3	0.0%	0.0%	0.0%
2,4-dichlorotoluene	205-970-0	256-96-2	256962	2444	Reach_1217	2009	3.58	0.25	3				-6.1	-5.8	-7.4	0.0%	0.0%	0.0%
N,N,N',N'-tetrakis(2-hydroxypropyl)adipamide	260-982-3	57843-53-5	57843535	3238	Reach_2827	2010	5.44	0.47	3	4.44	0.47		-4.8	-5.8	-7.5	0.0%	0.0%	0.0%
methylsilanetriyl triacetate	224-221-9	4253-34-3	4253343	2896	Reach_2023	2011	5.65	0.90	3	4.66	0.59		-6.0	-5.8	-7.4	0.0%	0.0%	0.0%
2-methylpentane-1,5-diamine	239-556-6	15520-10-2	15520102	2040	Reach_2390	2012	5.00	0.77	3	4.00	0.77		-6.0	-5.8	-7.5	0.0%	0.0%	0.0%
609-063-4	609-063-4	35113-48-5	35113485	2723	Reach_4288	2013	4.18	0.87	3				-6.0	-5.8	-7.4	0.0%	0.0%	0.0%
butyl 2-[[3-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carl	250-800-0	31778-10-6	31778106	2634	Reach_2657	2014	4.17	1.05	3	3.17	1.05		-5.6	-5.8	-7.4	0.0%	0.0%	0.0%
hexahydro-4,7-methano-1H-indenyl acrylate	223-032-9	3699-54-5	3699545	2788	Reach_1984	2015	6.46	0.61	3	5.46	0.61		-6.0	-5.8	-7.2	0.0%	0.0%	0.0%
diphenyl sulphone	204-853-1	127-63-9	127639	1813	Reach_1100	2016	4.40		2				-6.0	-5.8	-7.2	0.0%	0.0%	0.0%
tris(2-ethylhexyl) 2-(acetyloxy)propane-1,2,3-tricarboxylate	205-617-0	144-15-0	144150	1971	Reach_1193	2017	1.22	0.70	3	3.05			-5.8	-5.8	-6.3	0.0%	0.0%	0.0%
N,N'-hexane-1,6-diylbis[3-(3,5-di-tert-butyl-4-hydroxyphenylpro	245-442-7	23128-74-7	23128747	2345	Reach_2527	2018	4.78		2				-5.8	-5.8	-6.3	0.0%	0.0%	0.0%
ethylenebis(oxyethylene) bis[3-(5-tert-butyl-4-hydroxy-m-tolyl)p	253-039-2	36443-68-2	36443682	2767	Reach_2699	2019	5.27	0.45	3	4.27	0.45		-5.5	-5.8	-6.5	0.0%	0.0%	0.0%
2-fluorobenzoyl chloride	231-397-0	7531-52-4	7531524	3666	Reach_2259	2020	4.90	1.01	3				-6.0	-5.8	-7.1	0.0%	0.0%	0.0%
2-(2-oxoimidazolidin-1-yl)ethyl methacrylate	289-214-5	86261-90-7	86261907	3902	Reach_2989	2021	5.53	0.36	3	4.93	0.38		-4.9	-5.8	-7.5	0.0%	0.0%	0.0%
2-ethylaminoethanol	203-797-5	110-73-6	110736	282	Reach_826	2022	5.30	0.58	3	3.86	0.70		-5.9	-5.8	-7.4	0.0%	0.0%	0.0%
manganese, 4-[(5-chloro-4-methyl-2-sulfophenyl)azo]-3-hydroxy	226-102-7	5280-66-0	5280660	5916	Reach_2089	2023	5.11	0.45	3	3.94	0.90		-5.6	-5.8	-7.2	0.0%	0.0%	0.0%

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triethoxyoctylsilane	220-941-2	2943-75-1	2943751	2567	Reach_1891	2024	3.60	1.39	3	2.60	1.39		-6.1	-5.8	-7.1	0.0%	0.0%	0.0%
4-[(2,5-dichlorophenyl)azo]-N-(2,3-dihydro-2-oxo-1H-benzimidaz	230-258-1	6992-11-6	6992116	1287	Reach_2217	2025	4.17	1.05	3	3.17	1.05		-5.6	-5.8	-7.4	0.0%	0.0%	0.0%
3-methyl-1-(2,6,6-trimethylcyclohex-1-en-1-yl)penta-1,4-dien-3-	259-487-5	55117-15-2	55117152	3162	Reach_2805	2026							-5.9	-5.8	-7.2	0.0%	0.0%	0.0%
605-444-4	605-444-4	166524-64-7	166524647	2104	Reach_4174	2027	2.08	3.13	3				-5.0	-5.8	-7.4	0.0%	0.0%	0.0%
propylidynetrimethyl trimethacrylate	221-950-4	3290-92-4	3290924	2669	Reach_1942	2028	3.57	0.70	3	2.57	0.70		-6.0	-5.8	-7.4	0.0%	0.0%	0.0%
bis(2-ethylhexyl) fumarate	205-448-2	141-02-6	141026	1931	Reach_1155	2029	2.41	0.89	3	2.71			-5.9	-5.9	-7.5	0.0%	0.0%	0.0%
3-mercaptopropionic acid	203-537-0	107-96-0	107960	1473	Reach_723	2030	4.59	0.59	3	3.55	0.51		-5.0	-5.9	-7.5	0.0%	0.0%	0.0%
619-753-7	264-697-5	64131-85-7	64131857	3426	Reach_2864	2031	3.04	0.37	3				-5.1	-5.9	-7.5	0.0%	0.0%	0.0%
N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxo-2-[[2-(trifluor	268-734-6	68134-22-5	68134225	3507	Reach_2898	2032	4.17	1.01	3	3.17	1.01		-5.3	-5.9	-7.5	0.0%	0.0%	0.0%
2,4'-difluorobenzophenone	263-580-6	62518-65-4	62518654	3374	Reach_2854	2033	3.16	0.23	3				-6.1	-5.9	-7.2	0.0%	0.0%	0.0%
trifluoroacetyl chloride	206-556-2	354-32-5	354325	2732	Reach_1245	2034	4.80	0.56	3				-6.1	-5.9	-7.3	0.0%	0.0%	0.0%
(2Z)-but-2-ene-1,4-diyl diacetate	690-722-8	494799-36-9	494799369	2981	Reach_4659	2035	3.39	1.19	3				-6.0	-5.9	-7.3	0.0%	0.0%	0.0%
ethyl diphenylphosphinite	201-891-0	89-25-8	89258	3970	Reach_339	2036	1.87	2.93	3				-6.1	-5.9	-7.2	0.0%	0.0%	0.0%
616-466-9	265-512-0	65140-91-2	65140912	5971	Reach_2869	2037	5.46	0.20	3	4.46	0.20		-5.9	-5.9	-7.1	0.0%	0.0%	0.0%
5-methoxy-4-methyl-2,4-dihydro-3H-1,2,4-triazol-3-one	608-385-2	2963-69-1	2963691	2570	Reach_4274	2038	3.95	0.94	3				-4.9	-5.9	-7.5	0.0%	0.0%	0.0%
N,N'-ethane-1,2-diylbis(12-hydroxyoctadecan-1-amide)	204-613-6	123-26-2	123262	1765	Reach_1042	2039	4.83	0.55	3	3.83	0.55		-5.2	-5.9	-7.1	0.0%	0.0%	0.0%
2-ethylhexyl laurate	243-697-9	20292-08-4	20292084	2257	Reach_2491	2040	5.45	0.78	3	4.45	0.78		-5.7	-5.9	-7.1	0.0%	0.0%	0.0%
604-075-6	617-892-8	86604-75-3	86604753	6067	Reach_4478	2041	3.39	0.35	3	2.36	0.24		-5.6	-5.9	-7.0	0.0%	0.0%	0.0%
di-tert-butyl peroxide	203-733-6	110-05-4	110054	1514	Reach_803	2042	4.37		1	4.00			-6.1	-5.9	-8.2	0.0%	0.0%	0.0%
2,2′-dithiobis(5-ethoxy-7-fluoro[1,2,4]triazolo[1,5-c]pyrimidine)	695-187-4	166524-75-0	166524750	2108	Reach_4689	2043	4.73		2	5.10			-5.5	-5.9	-7.4	0.0%	0.0%	0.0%
3,3,5-trimethylcyclohexan-1-one	212-855-9	873-94-9	873949	3931	Reach_1582	2044	5.29		1				-6.1	-5.9	-7.0	0.0%	0.0%	0.0%
4-hydroxybutyl acrylate	219-606-3	2478-10-6	2478106	1247	Reach_1815	2045	4.22	0.12	3	3.40	0.23		-5.9	-5.9	-7.5	0.0%	0.0%	0.0%
3,7-dimethylocta-1,6-diene	219-433-3	2436-90-0	2436900	2390	Reach_1809	2046	3.20	0.06	3				-6.1	-5.9	-8.3	0.0%	0.0%	0.0%
α,α,α,2-tetrachlorotoluene	276-017-4	71786-67-9	71786679	6009	Reach_2931	2047	4.47		1				-6.1	-5.9	-7.2	0.0%	0.0%	0.0%
2-methoxy-4-(trifluoromethyl)pyridine-3-sulfonyl chloride	606-871-9	219715-41-0	219715410	2313	Reach_4223	2048	3.95	1.72	3				-6.0	-5.9	-7.3	0.0%	0.0%	0.0%
tetramethylene dimethacrylate	218-218-1	2082-81-7	2082817	2277	Reach_1756	2049	4.51	0.52	3	3.51	0.52		-6.0	-5.9	-7.4	0.0%	0.0%	0.0%
3-methoxy-3-methylbutan-1-ol	231-293-5	7486-38-6	7486386	6022	Reach_2255	2050	4.95	0.31	3	4.48	0.77		-6.1	-5.9	-7.4	0.0%	0.0%	0.0%
1-naphthyl isocyanate	201-703-7	86-84-0	86840	3911	Reach_304	2051	4.10	0.81	3				-6.1	-5.9	-7.2	0.0%	0.0%	0.0%
bis(2-ethylhexyl) tetrabromophthalate	247-426-5	26040-51-7	26040517	2450	Reach_2574	2052	-0.82	1.81	3	3.00			-6.0	-5.9	-6.3	0.0%	0.0%	0.0%
(S)-pyrrolidine-2-carboxamide	618-525-4	90315-82-5	90315825	3998	Reach_4496	2053	4.11	0.80	3				-5.1	-5.9	-7.5	0.0%	0.0%	0.0%
(R)-[[[(4-ethyl-2,3-dioxopiperazin-1-yl)carbonyl]amino]phenylace	243-248-7	19719-28-9	19719289	2238	Reach_2483	2054	5.00		2				-5.0	-5.9	-7.5	0.0%	0.0%	0.0%
2-[[[(3-amino-4-hydroxyphenyl)sulphonyl]amino]benzoic acid	603-434-4	130755-46-3	130755463	1842	Reach_4120	2055	2.39	1.16	3	1.39	1.16		-5.0	-5.9	-7.5	0.0%	0.0%	0.0%
potassium 3-sulphonatopropyl acrylate	250-465-0	31098-20-1	31098201	5837	Reach_2652	2056	4.86	1.05	3	3.86	1.05		-5.6	-5.9	-7.2	0.0%	0.0%	0.0%
N,N''-hexane-1,6-diylbis[N'-benzylurea]	254-274-3	39072-70-3	39072703	2833	Reach_2722	2057	3.12	0.55	3				-5.2	-5.9	-7.3	0.0%	0.0%	0.0%
butyl isocyanate	203-862-8	111-36-4	111364	298	Reach_853	2058	4.62	0.48	4	3.86	0.65		-6.1	-5.9	-7.2	0.0%	0.0%	0.0%
isopropenyl acetate	203-562-7	108-22-5	108225	1478	Reach_735	2059	4.32	0.22	3	3.32	0.22		-6.1	-5.9	-7.3	0.0%	0.0%	0.0%
1,8-diazabicyclo[5.4.0]undec-7-ene	201-849-1	88-66-4	88664	3962	Reach_328	2060	4.89		2				-6.1	-5.9	-7.2	0.0%	0.0%	0.0%
617-343-2	209-947-6	598-72-1	598721	3291	Reach_1405	2061	5.72	0.44	3				-6.1	-5.9	-7.2	0.0%	0.0%	0.0%
2-ethoxyethylamine	204-223-6	117-96-4	117964	5277	PharmaUBA	2062	3.82	0.74	3				-6.1	-5.9	-7.1	0.0%	0.0%	0.0%
3-(isodecyloxy)propylamine	259-265-8	54634-94-5	54634945	3149	Reach_2801	2063	3.04	0.16	3				-6.1	-5.9	-7.2	0.0%	0.0%	0.0%
N,N'-(2,5-dimethyl-1,4-phenylene)bis[3-oxobutyramide]	201-321-0	81-07-2	81072	98	Reach_270	2064	5.37	1.02	3	4.37	1.02		-5.0	-5.9	-7.4	0.0%	0.0%	0.0%
609-057-1	290-823-3	90268-23-8	90268238	3995	Reach_2991	2065	5.26	1.21	3	4.26	1.21		-5.6	-5.9	-7.2	0.0%	0.0%	0.0%
3,5-dimethylpyridine	209-708-6	591-22-0	591220	3266	Reach_1390	2066	4.19	0.62	3				-6.0	-5.9	-7.4	0.0%	0.0%	0.0%
manganese, 4-[(4-chloro-5-methyl-2-sulfophenyl)azo]-3-hydroxy	235-471-3	12238-31-2	12238312	5629	Reach_2310	2067	5.11	0.45	3	3.94	0.90		-5.6	-5.9	-7.2	0.0%	0.0%	0.0%
3',4',5'-trifluorobiphenyl-2-amine	220-358-3	2736-23-4	2736234	2501	Reach_1860	2068	4.22	1.12	3				-5.3	-5.9	-7.6	0.0%	0.0%	0.0%
1,5-dichloro-2-(1-methylethoxy)-4-nitrobenzene	255-259-4	41200-97-9	41200979	2872	Reach_2740	2069	3.24	0.48	3				-6.1	-5.9	-7.3	0.0%	0.0%	0.0%
1,1-diphenylethylene	608-371-6	29518-11-4	29518114	2568	Reach_4273	2070	4.33	1.25	3				-6.1	-5.9	-7.1	0.0%	0.0%	0.0%
dichloro(phenyl)phosphine	211-425-8	644-97-3	644973	3437	Reach_1480	2071	4.37	0.21	3				-6.1	-5.9	-7.0	0.0%	0.0%	0.0%
nonanoic acid	203-931-2	112-05-0	112050	320	Reach_886	2072	4.81	0.47	8	4.11	0.13		-5.9	-5.9	-7.5	0.0%	0.0%	0.0%
pyridine-2,3-dicarboxylic acid	605-637-3	172529-93-0	172529930	2128	Reach_4181	2073	5.16	0.59	3	4.16	0.59		-5.0	-5.9	-7.5	0.0%	0.0%	0.0%
butyric anhydride	203-383-4	106-31-0	106310	1434	Reach_664	2074	5.09	0.58	3	4.44	0.56		-6.1	-5.9	-7.2	0.0%	0.0%	0.0%
N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-2-[(2-methoxyphen	603-373-3	129909-90-6	129909906	415	Reach_4117	2075	3.70	1.58	12	3.39	0.67	5	-5.2	-5.9	-7.5	0.0%	0.0%	0.0%
phthalide	700-156-6	106649-95-0	106649950	5600	Reach_4783	2076							-5.8	-5.9	-7.5	0.0%	0.0%	0.0%
diiodohydroxyquinoline	206-001-4	281-23-2	281232	579	Reach_1220	2077	2.45	0.70	4	1.45	0.70		-5.6	-5.9	-7.4	0.0%	0.0%	0.0%
bis(2,6-diisopropylphenyl)carbodiimide	218-487-5	2162-74-5	2162745	2300	Reach_1767	2078	2.34	1.18	3	1.34	1.18		-5.8	-5.9	-6.6	0.0%	0.0%	0.0%
618-251-5	244-859-1	22235-81-0	22235810	2323	Reach_2519	2079	3.95	0.73	3				-4.9	-5.9	-7.5	0.0%	0.0%	0.0%
2-(2-ethoxyethoxy)ethyl acetate	203-940-1	112-15-2	112152	1577	Reach_890	2080	5.44	0.32	3	4.44	0.32		-6.1	-5.9	-7.5	0.0%	0.0%	0.0%
bis(2-(2-butoxyethoxy)ethyl) adipate	205-465-5	141-17-3	141173	1933	Reach_1158	2081	4.60	0.90	3	3.66	0.90		-6.0	-5.9	-7.4	0.0%	0.0%	0.0%
605-446-5	605-446-5	166524-74-9	166524749	2107	Reach_4175	2082							-5.3	-5.9	-7.4	0.0%	0.0%	0.0%
(3R)-3-aminobutan-1-ol	201-836-0	88-50-6	88506	3958	Reach_325	2083	4.19	0.77	3				-6.0	-5.9	-7.5	0.0%	0.0%	0.0%
2,2'-[(2,2',5,5'-tetrachloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-	244-776-0	22094-93-5	22094935	2317	Reach_2516	2084	5.26	1.21	3	4.26	1.21		-5.8	-5.9	-6.7	0.0%	0.0%	0.0%
2,3-epoxypropyl o-tolyl ether	218-645-3	2210-79-9	2210799	2319	Reach_1771	2085	3.87	0.29	3	2.87	0.29		-6.1	-5.9	-7.4	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl 4-(2-hydroxypropan-2-yl	241-621-9	17637-11-5	17637115	2146	Reach_2439	2086	5.24	1.47	3				-6.1	-5.9	-7.4	0.0%	0.0%	0.0%
5-Amino-2,4-di-tert-butylphenyl methyl carbonate	604-106-3	139007-06-0	139007060	1915	Reach_4141	2087	4.62	0.33	3	3.62	0.33		-5.6	-5.9	-7.4	0.0%	0.0%	0.0%
(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)(ethoxyimino)acetic acid	619-518-9	18480-53-0	18480530	2193	Reach_4527	2088	4.57	0.28	3				-5.2	-5.9	-7.5	0.0%	0.0%	0.0%
3,4-dichlorobenzonitrile	229-494-8	6574-99-8	6574998	3456	Reach_2194	2089	4.46		1				-6.1	-5.9	-7.0	0.0%	0.0%	0.0%
thiophene-2-ethylamine	230-947-7	7379-51-3	7379513	3626	Reach_2243	2090	3.89		2				-6.1	-5.9	-7.2	0.0%	0.0%	0.0%
1H-imidazole-1-propylamine	272-701-1	68909-32-0	68909320	3530	Reach_2912	2091	2.40	0.31	3				-5.1	-5.9	-7.6	0.0%	0.0%	0.0%
Ethyl 4-(2-hydroxypropan-2-yl)-2-propyl-1H-imidazole- 5-carbox	619-880-8	176972-62-6	176972626	2151	Reach_4552	2092	3.44	1.13	3				-5.2	-5.9	-7.5	0.0%	0.0%	0.0%
ethyl 4-hydroxybenzoate	204-399-4	120-47-8	120478	14	Reach_995	2093	4.23	0.17	3	3.39	0.34		-5.7	-5.9	-7.4	0.0%	0.0%	0.0%
octabenzone	217-421-2	1843-05-6	1843056	2191	Reach_1725	2094	4.72		1				-5.6	-5.9	-6.9	0.0%	0.0%	0.0%
(4aR,7S,8aR)-9,9-dimethyltetrahydro-4a,7-methanooxazireno[3,	202-384-7	95-02-3	95023	4117	Reach_421	2095	4.85		1				-5.5	-5.9	-7.4	0.0%	0.0%	0.0%
605-999-2	250-099-1	30246-33-4	30246334	2589	Reach_2644	2096	4.17	1.36	3				-5.2	-5.9	-7.5	0.0%	0.0%	0.0%
(2-hydroxy-3-sulphopropyl)dimethyl[3-[(1-oxododecyl)amino]pr	242-893-1	19223-55-3	19223553	5755	Reach_2475	2097	4.26		2	3.51			-5.6	-5.9	-7.3	0.0%	0.0%	0.0%
2,2,4(or 2,4,4)-trimethylhexanedinitrile	800-052-1	1421439-99-7	1421439997	5693	Reach_5036	2098							-6.0	-5.9	-7.4	0.0%	0.0%	0.0%
4,4'-methylenebis(2,6-xylidine)	244-912-9	22326-31-4	22326314	2329	Reach_2522	2099	6.10	0.68	3				-5.5	-5.9	-7.4	0.0%	0.0%	0.0%
methyl 3-{1,4-dioxaspiro[4.5]dec-8-yl[(trans-4-methylcyclohexyl	219-281-8	2402-77-9	2402779	2366	Reach_1795	2100	2.96	0.97	3				-5.5	-5.9	-7.1	0.0%	0.0%	0.0%
decan-4-olide	211-892-8	706-14-9	706149	813	Reach_1518	2101	4.19	0.43	4	3.35	0.60		-6.1	-5.9	-7.2	0.0%	0.0%	0.0%
606-548-2	611-869-6	59721-67-4	59721674	3285	Reach_4366	2102	3.35	0.11	3				-5.2	-5.9	-7.5	0.0%	0.0%	0.0%
3α,7α-dihydroxy-12-oxo-5β-cholan-24-oic acid	218-561-7	2182-55-0	2182550	2306	Reach_1769	2103	4.40	0.19	3	3.40	0.19		-5.4	-5.9	-7.5	0.0%	0.0%	0.0%
3-(1-cyanoethyl)benzoyl chloride	219-535-8	2457-01-4	2457014	5578	Reach_1812	2104	5.34	0.54	4	3.89	0.39		-6.1	-5.9	-7.4	0.0%	0.0%	0.0%
cis-hex-3-en-1-ol	213-192-8	928-96-1	928961	1016	Reach_1602	2105	5.50	0.10	3	4.50	0.10		-6.1	-5.9	-7.1	0.0%	0.0%	0.0%
2,2,4-trimethylpentane	208-759-1	540-84-1	540841	3122	Reach_1335	2106	3.25	0.62	3	2.25	0.62		-6.1	-5.9	-8.4	0.0%	0.0%	0.0%
8-chlorotheophylline	201-590-4	85-18-7	85187	3883	Reach_292	2107	3.34	1.97	3				-5.0	-5.9	-7.5	0.0%	0.0%	0.0%
α-ethyl-p-methoxybenzyl alcohol	226-315-5	5349-60-0	5349600	3104	Reach_2101	2108	4.37	0.31	3				-5.9	-5.9	-7.5	0.0%	0.0%	0.0%
3,4-dichlorophenyl isocyanate	211-790-3	696-23-1	696231	3545	Reach_1511	2109	3.99	0.80	3				-6.1	-5.9	-7.0	0.0%	0.0%	0.0%
(E)-3-formylbut-2-enyl acetate	247-825-4	26586-02-7	26586027	2480	Reach_2589	2110	3.98	0.22	3	3.18	0.35		-6.1	-5.9	-7.5	0.0%	0.0%	0.0%
3-(triethoxysilyl)propanethiol	279-914-9	82199-12-0	82199120	3820	Reach_2963	2111	4.17	1.01	3	3.17	1.01		-6.1	-5.9	-7.2	0.0%	0.0%	0.0%
hexamethylcyclotrisiloxane	208-765-4	541-05-9	541059	3126	Reach_1339	2112	5.74	0.60	3	3.24	1.04		-6.2	-5.9	-8.0	0.0%	0.0%	0.0%
malic acid	230-022-8	6915-15-7	6915157	3533	Reach_2210	2113	5.38		1				-4.9	-5.9	-7.6	0.0%	0.0%	0.0%
2,2-dimethylpropane-1,3-diyl cyclohex-4-ene-1,2-dicarboxylate	255-180-5	41026-17-9	41026179	2868	Reach_2733	2114	4.52		1				-5.4	-5.9	-7.5	0.0%	0.0%	0.0%
3,6,9-trioxaundecane-1,11-diol	203-989-9	112-60-7	112607	1594	Reach_915	2115	5.50		3	4.50			-5.0	-5.9	-7.6	0.0%	0.0%	0.0%
2,2,6,6-tetramethyl-4-oxopiperidinooxy	220-778-7	2896-70-0	2896700	2550	Reach_1881	2116	5.29	0.21	3	4.29	0.21		-5.1	-5.9	-7.5	0.0%	0.0%	0.0%
pentan-1-ol	246-349-4	24605-36-5	24605365	5791	Reach_2550	2117							-6.1	-5.9	-7.3	0.0%	0.0%	0.0%
N,N'-bis(3-aminopropyl)ethylenediamine	234-147-9	10563-26-5	10563265	1417	Reach_2297	2118	5.31	0.27	3	4.31	0.27		-5.1	-5.9	-7.7	0.0%	0.0%	0.0%
methyl 4-acetamido-5-iodo-2-methoxybenzoate	607-206-5	23175-18-0	23175180	2346	Reach_4235	2119	3.86	0.69	3				-5.4	-5.9	-7.4	0.0%	0.0%	0.0%
N,N'-(methylenedi-p-phenylene)bis[hexahydro-2-oxo-1H-azepin	258-981-8	54112-23-1	54112231	3127	Reach_2797	2120	3.27	0.57	3				-5.2	-5.9	-7.4	0.0%	0.0%	0.0%
N,N-dimethylacrylamide	220-237-5	2680-03-7	2680037	1254	Reach_1852	2121	5.55	0.23	3	4.55	0.23		-6.1	-5.9	-7.5	0.0%	0.0%	0.0%
5-chloro-2-nitrophenol	700-556-0	66682-07-3	66682073	3478	Reach_4933	2122	4.61		2				-5.8	-5.9	-7.5	0.0%	0.0%	0.0%
hydroxycyclohexyl phenyl ketone	213-426-9	947-19-3	947193	4112	Reach_1616	2123	4.41	0.53	3	3.52	0.83		-5.8	-5.9	-7.5	0.0%	0.0%	0.0%
619-293-7	700-069-3	265136-65-0	265136650	2473	Reach_4750	2124							-5.2	-5.9	-7.5	0.0%	0.0%	0.0%
1-(2-hydroxyethyl)imidazolidin-2-one	208-807-1	542-28-9	542289	3136	Reach_1347	2125	4.39	0.93	3				-5.1	-5.9	-7.6	0.0%	0.0%	0.0%
dibutyl hydrogen phosphate	203-509-8	107-66-4	107664	1467	Reach_713	2126	5.02	0.22	3	4.02	0.22		-5.3	-5.9	-7.6	0.0%	0.0%	0.0%
4,4'-dinitrostilbene-2,2'-disulphonic acid	204-885-6	128-42-7	128427	1821	Reach_1110	2127	5.50	1.12	3				-5.0	-5.9	-7.7	0.0%	0.0%	0.0%
2,2,4(or 2,4,4)-trimethyladipic acid	255-679-8	42142-52-9	42142529	2890	Reach_2750	2128	4.10	0.80	3				-5.3	-5.9	-7.5	0.0%	0.0%	0.0%
601-722-4	601-722-4	120570-77-6	120570776	1716	Reach_4102	2129	5.14	0.30	3	4.14	0.30		-6.1	-5.9	-7.6	0.0%	0.0%	0.0%
2-aminopropane-1,3-diol	208-584-0	534-03-2	534032	3100	Reach_1331	2130	5.96	0.83	3	4.96	0.83		-5.3	-5.9	-7.6	0.0%	0.0%	0.0%
cyclohexylurea	211-822-6	698-90-8	698908	3551	Reach_1514	2131	4.33	1.29	3				-5.8	-5.9	-7.5	0.0%	0.0%	0.0%
methyl formylphenylacetate	201-975-7	90-20-0	90200	3993	Reach_361	2132	4.93	1.15	3				-5.7	-5.9	-7.5	0.0%	0.0%	0.0%
2,2',6,6'-tetra-tert-butyl-4,4'-methylenediphenol	204-279-1	118-82-1	118821	1679	Reach_971	2133	1.22	2.85	3	0.22	2.85		-5.6	-5.9	-6.5	0.0%	0.0%	0.0%
Methyl 3-amino-4-methylbenzoate	207-692-5	488-98-2	488982	2978	Reach_1294	2134	3.17	0.67	3				-5.3	-5.9	-7.5	0.0%	0.0%	0.0%
m-(1-cyanoethyl)benzoic acid	700-389-3	20208-39-3	20208393	2254	Reach_4884	2135	3.53	0.30	3				-5.3	-5.9	-7.5	0.0%	0.0%	0.0%
3-chloropropionic acid	203-534-4	107-94-8	107948	1471	Reach_721	2136	5.04		1	5.84			-5.1	-5.9	-7.5	0.0%	0.0%	0.0%
1-(N,N-bis(2-hydroxyethyl)amino)propan-2-ol	229-764-5	6712-98-7	6712987	3486	Reach_2204	2137	5.45	0.12	3	4.45	0.12		-5.1	-5.9	-7.6	0.0%	0.0%	0.0%
ethyl 2-cyano-3-ethoxyacrylate	202-624-0	97-97-2	97972	4176	Reach_492	2138	5.00		1				-6.1	-5.9	-7.5	0.0%	0.0%	0.0%
2,2'-isopropylidenebis(p-phenyleneoxy)diethanol	605-955-2	181997-72-8	181997728	2174	Reach_4186	2139	4.04	0.97	3				-5.3	-5.9	-7.4	0.0%	0.0%	0.0%
tributylamine	203-058-7	102-82-9	102829	156	Reach_600	2140	4.42	0.62	4	3.43	0.70		-6.2	-5.9	-7.4	0.0%	0.0%	0.0%
2-tert-butylhydroquinone	217-752-2	1948-33-0	1948330	523	Reach_1737	2141	2.57	0.45	7	1.57	0.45		-6.0	-5.9	-6.9	0.0%	0.0%	0.0%
609-262-6	609-262-6	36589-61-4	36589614	5860	Reach_4295	2142							-5.7	-5.9	-7.3	0.0%	0.0%	0.0%
Diammonium 5-(hexylsulfonyl)-2-{[3-methyl-2,7-dioxo-1-(3-sulfo	700-712-8	1054448-65-5	1054448655	5595	Reach_4975	2143	5.50		3	4.50			-5.7	-5.9	-7.3	0.0%	0.0%	0.0%
tetrabromophthalic anhydride	211-185-4	632-79-1	632791	3396	Reach_1473	2144	4.02		1	3.14			-5.8	-5.9	-7.3	0.0%	0.0%	0.0%
warfarin	216-731-5	1655-07-8	1655078	2100	Reach_1705	2145	5.27		2				-5.3	-5.9	-7.5	0.0%	0.0%	0.0%
propyloxirane	213-701-3	1003-14-1	1003141	1299	Reach_1633	2146	5.41	0.39	3	4.41	0.39		-6.2	-5.9	-7.5	0.0%	0.0%	0.0%
(3-chloropropyl)dimethoxymethylsilane	242-056-0	18171-19-2	18171192	2172	Reach_2455	2147	5.20	0.43	3	4.20	0.43		-6.2	-5.9	-7.4	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
6,6'-di-tert-butyl-4,4'-butylidenedi-m-cresol	201-618-5	85-60-9	85609	3893	Reach_298	2148	4.20		1				-5.7	-5.9	-6.4	0.0%	0.0%	0.0%
lauroyl chloride	203-941-7	112-16-3	112163	1578	Reach_891	2149	3.64	0.82	3	3.46	0.98		-6.2	-5.9	-8.0	0.0%	0.0%	0.0%
1,2-dimethoxyethane	203-794-9	110-71-4	110714	1528	Reach_825	2150	6.92	0.30	3	5.92	0.30		-6.2	-5.9	-7.1	0.0%	0.0%	0.0%
600-593-1	700-509-4	19294-29-2	19294292	5756	Reach_4915	2151							-5.3	-5.9	-7.5	0.0%	0.0%	0.0%
1,2-dimethylimidazole	700-555-5	1233733-31-7	1233733317	5633	Reach_4932	2152	5.57	0.10	3	4.57	0.10		-6.1	-5.9	-7.4	0.0%	0.0%	0.0%
thiodiethylene bis[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propiona	255-392-8	41484-35-9	41484359	2878	Reach_2743	2153	4.14		2				-6.0	-5.9	-6.4	0.0%	0.0%	0.0%
2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol	248-908-8	28219-61-6	28219616	2525	Reach_2615	2154	3.14	0.25	3	2.25	0.14		-6.0	-5.9	-7.3	0.0%	0.0%	0.0%
methylhydrazine	200-471-4	60-34-4	60344	752	Reach_58	2155	2.94	0.79	8	1.94	0.79		-6.1	-5.9	-7.5	0.0%	0.0%	0.0%
3-methoxybutan-1-ol	219-741-8	2517-43-3	2517433	2422	Reach_1827	2156	5.74	0.51	3				-6.1	-5.9	-7.5	0.0%	0.0%	0.0%
cytosine	800-303-5	1083057-14-0	1083057140	1482	Reach_5043	2157	3.72	0.31	3				-5.1	-5.9	-7.5	0.0%	0.0%	0.0%
(3,4-diethoxyphenyl)acetonitrile	218-849-2	2253-52-3	2253523	2335	Reach_1780	2158	4.96		1				-6.1	-5.9	-7.4	0.0%	0.0%	0.0%
methacrylonitrile	204-817-5	126-98-7	126987	1809	Reach_1093	2159	5.01	0.57	3	4.17	0.92		-6.2	-5.9	-7.0	0.0%	0.0%	0.0%
603-436-5	214-230-6	1115-70-4	1115704	5607	Reach_1649	2160				4.29			-5.2	-5.9	-7.5	0.0%	0.0%	0.0%
dimethyl glutarate	214-277-2	1119-40-0	1119400	1564	Reach_1654	2161	5.26		1				-6.1	-5.9	-7.5	0.0%	0.0%	0.0%
meglumine	203-977-3	112-49-2	112492	330	Reach_909	2162	7.20	0.17	4	6.20	0.17		-5.2	-5.9	-7.4	0.0%	0.0%	0.0%
(Z)-cyclooctene	201-944-8	89-83-8	89838	996	Reach_353	2163	3.94	0.84	48	2.94	0.84		-6.2	-5.9	-8.2	0.0%	0.0%	0.0%
2,4-dichlorophenylacetic acid	613-982-6	66742-57-2	66742572	3482	Reach_4393	2164	2.56	1.90	3				-5.4	-5.9	-7.5	0.0%	0.0%	0.0%
tris(oxiranylmethyl) benzene-1,2,4-tricarboxylate	230-638-7	7237-83-4	7237834	3604	Reach_2233	2165	4.23		2				-5.1	-5.9	-7.7	0.0%	0.0%	0.0%
N-[4-(aminocarbonyl)phenyl]-4-[[1-[[(2,3-dihydro-2-oxo-1H-benz	202-485-6	96-17-3	96173	1046	Reach_452	2166	4.21	0.52	3	3.21	0.52		-5.3	-5.9	-7.5	0.0%	0.0%	0.0%
5-ethyl-1,3-dioxane-5-methanol	225-967-8	5187-23-5	5187235	3048	Reach_2083	2167	6.43		1				-6.1	-5.9	-7.5	0.0%	0.0%	0.0%
propylamine	203-462-3	107-10-8	107108	208	Reach_693	2168	4.76	1.46	6	3.29	0.70		-6.2	-5.9	-6.9	0.0%	0.0%	0.0%
Cuprate(4-), [2-[[[[2-hydroxy-3-sulfo-5-[[2-(sulfooxy)ethyl]sulfon	291-103-1	90341-71-2	90341712	6079	Reach_2993	2169	5.06	0.88	3	4.06	0.88		-5.7	-6.0	-7.3	0.0%	0.0%	0.0%
dimethyl propylphosphonate	242-555-3	18755-43-6	18755436	2206	Reach_2468	2170	5.47		3	4.47			-6.1	-6.0	-7.3	0.0%	0.0%	0.0%
2,4,6,8-tetramethylcyclotetrasiloxane	219-137-4	2370-88-9	2370889	2355	Reach_1786	2171	8.24	0.65	3	7.24	0.65		-6.2	-6.0	-7.5	0.0%	0.0%	0.0%
2,6-di-tert-butyl-4-(4,6-bis(octylthio)-1,3,5-triazin-2-ylamino)phe	213-590-1	991-84-4	991844	4197	Reach_1625	2172	5.31	0.24	3	4.31	0.24		-6.1	-6.0	-6.4	0.0%	0.0%	0.0%
p-isopropylphenyl isocyanate	229-959-5	6860-97-5	6860975	3521	Reach_2209	2173	3.47	2.55	3				-6.2	-6.0	-7.0	0.0%	0.0%	0.0%
diethyl [2-(2,4-difluorophenyl)prop-2-en-1-yl]malonate	200-090-3	51-34-3	51343	3036	Reach_15	2174	4.64	0.95	3				-6.2	-6.0	-7.3	0.0%	0.0%	0.0%
allantoin	202-592-8	97-59-6	97596	4166	Reach_481	2175	5.92	2.01	3				-4.9	-6.0	-7.7	0.0%	0.0%	0.0%
4-chlorophthalic anhydride	211-754-7	693-57-2	693572	3540	Reach_1508	2176	5.09	0.51	3	4.09	0.51		-6.2	-6.0	-7.3	0.0%	0.0%	0.0%
Androsta-4,9(11)-diene-3,17-dione	616-391-1	76812-02-7	76812027	3725	Reach_4438	2177	1.76	1.37	3				-6.0	-6.0	-7.4	0.0%	0.0%	0.0%
620-037-1	617-458-8	83393-23-1	83393231	6048	Reach_4464	2178							-6.2	-6.0	-7.2	0.0%	0.0%	0.0%
(S)-(+)-1-methoxy-2-propylamine	617-448-3	83196-56-9	83196569	3842	Reach_4462	2179	3.05	0.15	3				-6.2	-6.0	-7.2	0.0%	0.0%	0.0%
succinimide	204-635-6	123-56-8	123568	1771	Reach_1053	2180	6.94		1				-5.1	-6.0	-7.7	0.0%	0.0%	0.0%
dicyclohexyl phthalate	201-545-9	84-61-7	84617	3871	Reach_286	2181	3.01	0.25	3	2.51			-5.7	-6.0	-7.1	0.0%	0.0%	0.0%
2-(2-chloroethoxy)ethanol	211-059-9	628-89-7	628897	3380	Reach_1461	2182	6.02	0.44	3	5.02	0.44		-5.9	-6.0	-7.5	0.0%	0.0%	0.0%
2-ethylhexylamine	203-233-8	104-75-6	104756	169	Reach_628	2183	4.02	0.59	5	2.82	0.70		-6.2	-6.0	-7.5	0.0%	0.0%	0.0%
methyl 4-hydroxybenzoate	202-785-7	99-76-3	99763	4216	Reach_538	2184	4.73	0.28	3	3.78	0.41		-5.9	-6.0	-7.5	0.0%	0.0%	0.0%
4-bromo-1,2-dichlorobenzene	607-674-0	25260-60-0	25260600	2425	Reach_4247	2185	3.55	0.85	3				-6.2	-6.0	-7.5	0.0%	0.0%	0.0%
[3R-(3α,3aβ,7β,8aα)]-1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramet	202-377-9	94-96-2	94962	1024	Reach_420	2186	5.73	0.40	3	4.73	0.40		-6.1	-6.0	-7.3	0.0%	0.0%	0.0%
L-proline	205-702-2	147-85-3	147853	1999	Reach_1197	2187	4.27	1.01	3	3.27	1.01		-4.9	-6.0	-7.6	0.0%	0.0%	0.0%
603-266-1	212-079-0	760-23-6	760236	870	Reach_1530	2188	4.20	0.27	4	3.43	0.24		-5.4	-6.0	-7.4	0.0%	0.0%	0.0%
methyl chloroacetate	202-501-1	96-34-4	96344	4145	Reach_463	2189	3.64	0.64	3	2.64	0.64		-6.1	-6.0	-7.3	0.0%	0.0%	0.0%
2-(diethylamino)-6-methyl-1H-pyrimidin-4-one	206-278-1	320-60-5	320605	2642	Reach_1234	2190	3.30	0.30	3				-5.3	-6.0	-7.5	0.0%	0.0%	0.0%
Disodium 4-amino-5-hydroxy-3,6-bis{(E)-[4-(vinylsulfonyl)phenyl	695-988-9	100556-82-9	100556829	5591	Reach_4699	2191	5.00	0.71	3	4.30	0.94		-5.7	-6.0	-7.3	0.0%	0.0%	0.0%
δ-valerolactone	236-143-2	13188-60-8	13188608	5664	Reach_2326	2192							-6.1	-6.0	-7.6	0.0%	0.0%	0.0%
octanal	225-625-8	4979-32-2	4979322	2990	Reach_2069	2193	3.39	0.65	3	2.68	1.30		-6.2	-6.0	-7.4	0.0%	0.0%	0.0%
hexanoic acid	205-550-7	142-62-1	142621	462	Reach_1179	2194	5.05	0.31	5	4.05	0.31		-5.8	-6.0	-7.6	0.0%	0.0%	0.0%
triethoxy(2,4,4-trimethylpentyl)silane	252-558-1	35435-21-3	35435213	2734	Reach_2690	2195	4.18	1.14	3	3.18	1.14		-6.2	-6.0	-7.3	0.0%	0.0%	0.0%
di(tert-butyl) carbonate	246-240-1	24424-99-5	24424995	2393	Reach_2545	2196	5.05	0.31	3	4.05	0.31		-6.2	-6.0	-7.2	0.0%	0.0%	0.0%
1-(2,4-dichlorophenyl)ethan-1-one	218-780-8	2234-16-4	2234164	541	Reach_1776	2197	4.07		2				-6.2	-6.0	-7.1	0.0%	0.0%	0.0%
(E)-anethole	224-052-0	4180-23-8	4180238	635	Reach_2019	2198	3.85	0.12	6	2.85	0.12		-6.2	-6.0	-7.1	0.0%	0.0%	0.0%
1,3-bis(isocyanatomethyl)benzene	222-852-4	3634-83-1	3634831	2766	Reach_1978	2199	4.55	0.46	3	3.55	0.46		-6.0	-6.0	-7.5	0.0%	0.0%	0.0%
2-methylpropane-2-thiol	200-890-2	75-66-1	75661	3679	Reach_157	2200	4.31	0.29	3	3.31	0.29		-6.2	-6.0	-8.0	0.0%	0.0%	0.0%
N-[3-(dimethylamino)propyl]stearamide	231-609-1	7651-02-7	7651027	1289	Reach_2266	2201	2.41	0.23	3	1.58	0.28		-5.6	-6.0	-6.9	0.0%	0.0%	0.0%
2,4-dichlorophenyl isocyanate	200-749-5	71-30-7	71307	3580	Reach_100	2202	3.99	1.29	3				-6.2	-6.0	-7.2	0.0%	0.0%	0.0%
dioctadecyl ether	228-567-1	6297-03-6	6297036	1281	Reach_2163	2203	6.51		1				-6.2	-6.0	-4.8	0.0%	0.0%	0.0%
3,7-dimethyloctan-3-ol	201-133-9	78-69-3	78693	3755	Reach_204	2204	4.22	0.18	3	3.46	0.18		-6.2	-6.0	-7.3	0.0%	0.0%	0.0%
tripropylamine	203-047-7	102-69-2	102692	154	Reach_595	2205	4.79	0.70	20	3.85	0.70		-6.2	-6.0	-7.4	0.0%	0.0%	0.0%
N-(2,6-difluorophenyl)-5-methyl[1,2,4]triazolo[1,5-a]pyrimidine-:	619-383-6	98967-40-9	98967409	1081	Reach_4516	2206	4.42	2.08	12	3.42	2.08		-5.5	-6.0	-6.8	0.0%	0.0%	0.0%
602-965-9	615-927-1	7319-16-6	7319166	3614	Reach_4419	2207	3.24	1.69	3				-6.2	-6.0	-7.4	0.0%	0.0%	0.0%
2-ethyl-2-[[(1-oxoheptyl)oxy]methyl]propane-1,3-diyl bisheptan	203-904-5	111-75-1	111751	1556	Reach_868	2208	4.83	0.74	3	3.67	0.96		-5.8	-6.0	-6.5	0.0%	0.0%	0.0%
4-bromophenyl acetate	217-668-6	1927-95-3	1927953	2229	Reach_1735	2209	3.88		1				-6.2	-6.0	-7.1	0.0%	0.0%	0.0%

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Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
di-sec-butylphenol, mixed isomers	226-854-6	5510-99-6	5510996	3160	Reach_2120	2210	2.64	0.32	3				-6.2	-6.0	-7.2	0.0%	0.0%	0.0%
2,2'-ethylenedioxydiethyl dimethacrylate	203-652-6	109-16-0	109160	1495	Reach_772	2211	4.93	0.61	3	3.93	0.61		-6.2	-6.0	-7.6	0.0%	0.0%	0.0%
602-890-1	602-890-1	122731-58-2	122731582	1757	Reach_4106	2212							-4.9	-6.0	-7.8	0.0%	0.0%	0.0%
687-796-9	235-557-0	12286-65-6	12286656	5631	Reach_2311	2213	3.69	1.39	3	2.69	1.39		-5.7	-6.0	-7.4	0.0%	0.0%	0.0%
calcium bis[3-nitro-4-[[2-oxo-1-[(phenylamino)carbonyl]propyl]a	200-795-6	73-22-3	73223	3616	Reach_106	2214	4.19	0.07	3				-5.7	-6.0	-7.4	0.0%	0.0%	0.0%
(E,E,E)-2,7-dimethylocta-2,4,6-trienedial	611-255-8	55314-16-4	55314164	3166	Reach_4354	2215	4.77	0.50	3	3.77	0.50		-6.2	-6.0	-7.6	0.0%	0.0%	0.0%
1-chlorooctane	203-915-5	111-85-3	111853	1561	Reach_876	2216	3.56	0.74	3	2.56	0.74		-6.2	-6.0	-8.4	0.0%	0.0%	0.0%
4-[[(2-aminophenyl)methyl]amino]cyclohexyl acetate	616-785-3	80012-43-7	80012437	3785	Reach_4444	2217	3.72	0.63	3				-5.4	-6.0	-7.6	0.0%	0.0%	0.0%
2,6-dichloro-N-(2,6-dimethylphenyl)hexanamide	200-385-7	58-55-9	58559	730	Reach_47	2218	5.17	0.37	3	4.17	0.37		-5.6	-6.0	-7.5	0.0%	0.0%	0.0%
1,3,5-triisopropyl-2,4-dinitrobenzene	247-578-2	26272-90-2	26272902	2460	Reach_2578	2219	3.38	1.13	3	2.38	1.13		-6.1	-6.0	-7.2	0.0%	0.0%	0.0%
619-511-0	244-104-6	20893-30-5	20893305	2280	Reach_2501	2220	3.72	0.90	3				-6.2	-6.0	-7.1	0.0%	0.0%	0.0%
2,6-dichlorotoluene	204-269-7	118-69-4	118694	1676	Reach_968	2221	3.80	0.36	3	2.80	0.36		-6.2	-6.0	-7.6	0.0%	0.0%	0.0%
5-methylhexan-2-one	203-737-8	110-12-3	110123	273	Reach_804	2222	5.46	0.46	3	4.32	0.32		-6.2	-6.0	-7.3	0.0%	0.0%	0.0%
2-methylbut-2-ene	208-156-3	513-35-9	513359	3033	Reach_1317	2223	3.78	0.22	3	2.78	0.22		-6.2	-6.0	-8.5	0.0%	0.0%	0.0%
(2,4,6-trioxotriazine-1,3,5(2H,4H,6H)-triyl)tris(hexamethylene) is	204-642-4	123-68-2	123682	1773	Reach_1055	2224	2.77	0.52	3	1.81	0.59		-5.9	-6.0	-6.4	0.0%	0.0%	0.0%
2,3-didehydro-D-erythro-hexono-1,4-lactone	201-928-0	89-65-6	89656	3982	Reach_349	2225	5.15		2				-4.9	-6.0	-7.7	0.0%	0.0%	0.0%
pentapotassium ({[(hydroxyphosphinato)methyl](phosphonaton	700-903-6	255830-15-0	255830150	2438	Reach_5021	2226	5.69		2	4.46			-6.2	-6.0	-7.2	0.0%	0.0%	0.0%
α,4-dichlorotoluene	700-275-3	718-71-8	718718	3593	Reach_4835	2227	2.89	0.73	3				-6.2	-6.0	-7.2	0.0%	0.0%	0.0%
di-tert-butyl 1,1,4,4-tetramethyltetramethylene diperoxide	201-128-1	78-63-7	78637	3753	Reach_202	2228	2.89	0.67	3	1.89	0.67		-6.2	-6.0	-8.2	0.0%	0.0%	0.0%
619-846-2	256-462-0	49744-39-0	49744390	5895	Reach_2765	2229							-6.1	-6.0	-7.4	0.0%	0.0%	0.0%
4H-3,1-benzoxazine-2,4(1H)-dione	202-209-4	93-01-6	93016	4055	Reach_396	2230	4.78	0.36	3				-6.0	-6.0	-7.5	0.0%	0.0%	0.0%
camphene	201-234-8	79-92-5	79925	928	Reach_251	2231	4.16	1.01	7	3.16	1.01		-6.3	-6.0	-8.0	0.0%	0.0%	0.0%
2-Butenoic acid, 4-oxo-4-(tridecylamino)-, (Z)-, branched	283-219-6	84583-68-6	84583686	3868	Reach_2976	2232	4.05	0.26	3	3.05	0.26		-5.5	-6.0	-7.6	0.0%	0.0%	0.0%
cyclohexyl isocyanate	212-958-9	887-76-3	887763	3964	Reach_1585	2233							-6.2	-6.0	-7.2	0.0%	0.0%	0.0%
8,9,10-trinorborn-2-ene	207-866-0	498-66-8	498668	650	Reach_1297	2234	4.01	0.19	3	3.01	0.19		-6.3	-6.0	-8.1	0.0%	0.0%	0.0%
(1R)-6,6-dimethylbicyclo[3.1.1]hept-2-en-2-ethanol	252-744-2	35836-73-8	35836738	2751	Reach_2694	2235	4.52	0.23	3				-6.2	-6.0	-7.5	0.0%	0.0%	0.0%
N,N-dicyclohexylbenzothiazole-2-sulphenamide	204-683-8	124-13-0	124130	1786	Reach_1070	2236	3.81	0.41	3	2.81	0.41		-6.2	-6.0	-8.2	0.0%	0.0%	0.0%
isosorbide dinitrate	201-740-9	87-33-2	87332	3926	Reach_308	2237	5.63	1.59	3				-5.4	-6.0	-7.7	0.0%	0.0%	0.0%
exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl methacrylate	231-403-1	7534-94-3	7534943	3668	Reach_2260	2238	3.18	0.20	3	2.27	0.35		-6.2	-6.0	-7.4	0.0%	0.0%	0.0%
4-tert-butylcyclohexanone	617-040-5	80286-58-4	80286584	3790	Reach_4445	2239	3.72	0.08	3				-6.2	-6.0	-7.2	0.0%	0.0%	0.0%
606-524-1	700-231-3	18162-90-8	18162908	2170	Reach_4814	2240							-5.5	-6.0	-7.4	0.0%	0.0%	0.0%
(3R,5aS,6R,8aS,9R,12S,12aR)-3,6,9-trimethyloctahydro-3,12-epo	209-939-2	598-55-0	598550	3290	Reach_1403	2241	5.02	1.27	3				-5.6	-6.0	-7.6	0.0%	0.0%	0.0%
(1S,4R,6R)-1-[(3E)-5-hydroxy-3-methylpent-3-en-1-yn-1-yl]-2,2,6	700-075-6	218768-11-7	218768117	2309	Reach_4753	2242	3.50	0.57	3				-5.4	-6.0	-7.5	0.0%	0.0%	0.0%
cinnamaldehyde	203-213-9	104-55-2	104552	168	Reach_623	2243	4.10	0.84	5	3.26	0.93		-6.2	-6.0	-7.3	0.0%	0.0%	0.0%
2-ethylhexyl salicylate	204-263-4	118-60-5	118605	1675	Reach_967	2244	3.33	1.80	3	2.33	1.80		-6.0	-6.0	-7.3	0.0%	0.0%	0.0%
vinyltoluene	246-562-2	25013-15-4	25013154	2412	Reach_2557	2245	3.44	0.27	3	2.44	0.27		-6.3	-6.0	-7.8	0.0%	0.0%	0.0%
1,2,3,4-tetrahydronaphthalene	204-340-2	119-64-2	119642	355	Reach_983	2246	3.75	0.70	16	3.07	0.70		-6.2	-6.0	-7.6	0.0%	0.0%	0.0%
616-291-8	616-291-8	76114-73-3	76114733	3699	Reach_4431	2247	5.12	0.31	3	4.12	0.31		-6.2	-6.0	-7.4	0.0%	0.0%	0.0%
2-(4-methylpentan-2-yl)aniline	615-161-8	707-72-2	707722	3569	Reach_4412	2248							-6.2	-6.0	-7.6	0.0%	0.0%	0.0%
3-(triethoxysilyl)propyl prop-2-enoate	258-011-3	52567-96-1	52567961	3063	Reach_2783	2249	4.25	0.55	3				-6.2	-6.0	-7.6	0.0%	0.0%	0.0%
acetoacetamide	227-774-4	5977-14-0	5977140	3286	Reach_2146	2250	7.00		1				-5.5	-6.0	-7.7	0.0%	0.0%	0.0%
616-320-4	616-320-4	763105-70-0	763105700	3708	Reach_4434	2251	2.20	3.12	3				-5.3	-6.0	-7.7	0.0%	0.0%	0.0%
2-ethylhexyl acetate	203-079-1	103-09-3	103093	1359	Reach_601	2252	4.37	0.42	3	3.37	0.42		-6.2	-6.0	-7.6	0.0%	0.0%	0.0%
tetradecanedioic acid	212-476-9	821-38-5	821385	3819	Reach_1554	2253	4.59		1				-5.6	-6.0	-7.6	0.0%	0.0%	0.0%
(E)-3-methylpent-2-en-4-yn-1-ol	690-510-5	5693-27-6	5693276	3216	Reach_4656	2254	4.46	0.93	3				-6.2	-6.0	-7.5	0.0%	0.0%	0.0%
(Z)-3-methylpent-2-en-4-yn-1-ol	611-622-2	581076-60-0	581076600	3241	Reach_4361	2255	2.51		1				-6.2	-6.0	-7.5	0.0%	0.0%	0.0%
2,4,6,8,10-pentamethylcyclopentasiloxane	228-204-7	6166-86-5	6166865	3347	Reach_2156	2256	8.24	0.65	3	7.24	0.65		-6.2	-6.0	-7.5	0.0%	0.0%	0.0%
2-ethylhexyl chloroformate	246-278-9	24468-13-1	24468131	2395	Reach_2547	2257	3.56	0.67	3	2.56	0.67		-6.3	-6.0	-8.0	0.0%	0.0%	0.0%
3-[methoxy(dimethyl)silyl]propan-1-amine	207-256-4	456-04-2	456042	2944	Reach_1280	2258	2.60		1				-6.2	-6.0	-7.4	0.0%	0.0%	0.0%
stearamide	204-693-2	124-26-5	124265	1789	Reach_1074	2259	2.52	0.28	3	1.52	0.28		-6.1	-6.0	-7.1	0.0%	0.0%	0.0%
1-[4-(trans-4-propylcyclohexyl)phenyl]butan-1-one	639-407-9	201733-56-4	201733564	2252	Reach_4604	2260							-5.8	-6.0	-7.1	0.0%	0.0%	0.0%
4,4'-diamino[1,1'-bianthracene]-9,9',10,10'-tetraone	223-754-4	4051-63-2	4051632	2858	Reach_2007	2261	2.80	0.21	3				-5.4	-6.0	-7.5	0.0%	0.0%	0.0%
N,N'-1,4-phenylenebis[3-oxobutyramide]	246-438-8	24731-73-5	24731735	2402	Reach_2554	2262	4.86	1.39	3				-5.1	-6.0	-7.6	0.0%	0.0%	0.0%
2-cyano-N-methylacetamide	690-730-1	486460-32-6	486460326	2974	Reach_4660	2263	3.82	1.81	3				-5.3	-6.0	-7.8	0.0%	0.0%	0.0%
3-α-hydroxy-7-oxo-5-β-cholan-24-oic acid	238-883-1	14814-09-6	14814096	2001	Reach_2370	2264	5.16	0.79	3	4.06	0.77		-5.5	-6.0	-7.6	0.0%	0.0%	0.0%
acetyl chloride	200-865-6	75-36-5	75365	858	Reach_141	2265	4.30	0.97	4	3.30	0.97		-6.3	-6.0	-7.9	0.0%	0.0%	0.0%
7-oxabicyclo[4.1.0]hept-3-ylmethyl 7-oxabicyclo[4.1.0]heptane-3	219-207-4	2386-87-0	2386870	2362	Reach_1792	2266	4.65	0.24	3	3.53	0.51		-6.2	-6.0	-7.6	0.0%	0.0%	0.0%
hexadecyl 2-ethylhexanoate	204-493-5	121-69-7	121697	373	Reach_1018	2267	4.66	0.52	11	3.66	0.73	33	-6.1	-6.0	-6.8	0.0%	0.0%	0.0%
tris(2-chloroethyl) phosphate	700-177-0	467430-13-3	467430133	5892	Reach_4792	2268							-6.2	-6.0	-6.9	0.0%	0.0%	0.0%
620-343-5	611-624-3	581076-67-7	581076677	5939	Reach_4362	2269	4.75	0.60	3	3.75	0.60		-6.2	-6.0	-7.2	0.0%	0.0%	0.0%
1-ethynylcyclohexanol	288-270-8	85702-79-0	85702790	3896	Reach_2987	2270	4.96	0.97	3	4.48	0.99		-6.3	-6.0	-7.0	0.0%	0.0%	0.0%
linalyl acetate	204-116-4	115-95-7	115957	1640	Reach_947	2271	4.43	0.40	3	3.61	0.30		-6.2	-6.0	-7.4	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
1,4-dihydroxyanthraquinone	229-942-2	6850-63-1	6850631	801	Reach_2208	2272	4.68	0.24	3	3.80	0.24		-5.4	-6.0	-7.5	0.0%	0.0%	0.0%
3,5,5-trimethylhexan-1-ol	222-376-7	3452-97-9	3452979	609	Reach_1964	2273	4.12	0.18	5	3.12	0.18		-6.3	-6.0	-7.2	0.0%	0.0%	0.0%
616-123-3	616-123-3	746595-79-9	746595799	3641	Reach_4423	2274	1.92	3.16	3				-5.3	-6.0	-7.7	0.0%	0.0%	0.0%
methyl 3-oxovalerate	202-299-5	94-05-3	94053	4097	Reach_411	2275	4.99		1				-6.2	-6.0	-7.5	0.0%	0.0%	0.0%
chloroacetone	201-161-1	78-95-5	78955	3761	Reach_218	2276	2.78		1				-6.3	-6.0	-7.2	0.0%	0.0%	0.0%
O,O-diisopropyl hydrogen dithiophosphate	221-496-7	3120-74-9	3120749	2620	Reach_1918	2277	3.69	0.32	3				-6.3	-6.0	-7.2	0.0%	0.0%	0.0%
nerol	203-378-7	106-25-2	106252	187	Reach_662	2278	4.18	0.35	3	3.03	0.47		-6.2	-6.0	-7.3	0.0%	0.0%	0.0%
3-methoxyandrosta-3,5-dien-17-one	220-371-4	2741-57-3	2741573	2505	Reach_1861	2279	2.92	0.72	3				-6.2	-6.0	-7.5	0.0%	0.0%	0.0%
dodecane-1-thiol	203-984-1	112-55-0	112550	1592	Reach_913	2280	3.41	1.33	3	2.41	1.33		-6.2	-6.0	-8.2	0.0%	0.0%	0.0%
(epoxyethyl)benzene	202-476-7	96-09-3	96093	1044	Reach_450	2281	4.19	0.33	6	3.19	0.33		-6.2	-6.0	-7.2	0.0%	0.0%	0.0%
methyl isothiocyanate	209-132-5	556-61-6	556616	704	Reach_1367	2282	2.27	0.80	33	1.29	0.80		-6.3	-6.0	-7.3	0.0%	0.0%	0.0%
2,2'-[ethane-1,2-diylbis(oxy)]bisethyl diacetate	203-846-0	111-21-7	111217	1542	Reach_849	2283	5.34	0.23	3	4.34	0.23		-5.8	-6.0	-7.8	0.0%	0.0%	0.0%
p-phenylbenzaldehyde	221-742-3	3218-36-8	3218368	2644	Reach_1934	2284	3.34	0.36	3				-6.2	-6.0	-7.4	0.0%	0.0%	0.0%
4-(trifluoromethoxy)aniline	207-317-5	461-82-5	461825	2949	Reach_1284	2285	3.71	0.54	3				-5.9	-6.0	-7.7	0.0%	0.0%	0.0%
(1-hydroxyethylidene)bisphosphonic acid, potassium salt	267-956-0	67953-76-8	67953768	5990	Reach_2893	2286	5.66		2	4.30			-5.8	-6.0	-7.4	0.0%	0.0%	0.0%
exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acetate	204-727-6	125-12-2	125122	1796	Reach_1083	2287	3.61	0.45	3	2.61	0.45		-6.3	-6.0	-7.4	0.0%	0.0%	0.0%
trichloro(propyl)silane	205-489-6	141-57-1	141571	1936	Reach_1164	2288	6.31	0.30	3	5.31	0.30		-6.3	-6.0	-7.5	0.0%	0.0%	0.0%
800-181-3	204-018-1	112-95-8	112958	1613	Reach_931	2289	7.67		1				-5.8	-6.0	-7.4	0.0%	0.0%	0.0%
manganese oxalate	211-367-3	640-67-5	640675	5965	Reach_1478	2290	4.92	0.41	3	3.92	0.41		-5.8	-6.0	-7.4	0.0%	0.0%	0.0%
isobutyl vinyl ether	203-678-8	109-53-5	109535	1501	Reach_775	2291	4.63	0.12	3	3.80	0.23		-6.3	-6.0	-8.0	0.0%	0.0%	0.0%
2-allyloxymethyl-2-ethylpropanediol	211-662-7	682-11-1	682111	3511	Reach_1500	2292	5.95	0.35	3	5.03	0.40		-5.4	-6.0	-7.7	0.0%	0.0%	0.0%
2,6-diisopropylphenyl isocyanate	201-869-0	88-95-9	88959	3965	Reach_334	2293	4.35	0.92	3				-6.3	-6.0	-7.3	0.0%	0.0%	0.0%
2-methylbutene	247-975-0	26760-64-5	26760645	2486	Reach_2592	2294	3.78	0.22	3	2.78	0.22		-6.3	-6.0	-8.4	0.0%	0.0%	0.0%
2,3,7,8-tetrahydro-2,5,8-benzotrioxacycloundecine-1,9-dione	205-491-7	141-62-8	141628	1939	Reach_1165	2295	1.38	0.41	3	0.38	0.41		-5.3	-6.0	-7.7	0.0%	0.0%	0.0%
α,2,2,6-tetramethylcyclohexene-1-butyraldehyde	206-524-8	352-70-5	352705	2727	Reach_1243	2296	4.10	0.37	3				-6.2	-6.0	-7.1	0.0%	0.0%	0.0%
propionic anhydride	204-638-2	123-62-6	123626	1772	Reach_1054	2297	4.65	0.21	3	3.65	0.21		-6.2	-6.0	-7.4	0.0%	0.0%	0.0%
p-menth-1-en-8-ol	202-680-6	98-55-5	98555	1074	Reach_512	2298	4.73	0.24	5	3.73	0.24		-6.3	-6.0	-7.5	0.0%	0.0%	0.0%
1,2,3-trichlorobenzene	207-677-3	488-43-7	488437	2977	Reach_1293	2299	6.43	1.32	3				-6.3	-6.0	-7.5	0.0%	0.0%	0.0%
2-chloro-1,1-dimethoxyethane	202-751-1	99-34-3	99343	4204	Reach_527	2300	5.01	0.81	3	4.01	0.81		-6.3	-6.0	-7.3	0.0%	0.0%	0.0%
2-methyl-6-methyleneoct-7-en-2-ol	208-843-8	543-39-5	543395	3138	Reach_1349	2301	3.96	0.15	3				-6.3	-6.0	-7.2	0.0%	0.0%	0.0%
trazodone	203-913-4	111-84-2	111842	1560	Reach_875	2302	2.89	0.47	3	1.89	0.47		-5.5	-6.1	-7.6	0.0%	0.0%	0.0%
3,3-bis[(dimethylvinylsilyl)oxy]-1,1,5,5-tetramethyl-1,5-divinyltri	262-061-1	60111-54-8	60111548	3304	Reach_2843	2303	0.70	3.06	3	-0.30	3.06		-6.2	-6.1	-6.9	0.0%	0.0%	0.0%
octane-1-thiol	203-918-1	111-88-6	111886	1563	Reach_879	2304	2.02	0.64	3	1.21	1.33		-6.3	-6.1	-7.9	0.0%	0.0%	0.0%
2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2-meth	224-867-1	4531-49-1	4531491	2939	Reach_2046	2305	5.26	1.21	3	4.26	1.21		-5.4	-6.1	-7.2	0.0%	0.0%	0.0%
605-152-7	212-562-6	826-81-3	826813	3836	Reach_1558	2306	4.06	0.27	3				-6.2	-6.1	-7.5	0.0%	0.0%	0.0%
exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acrylate	227-561-6	5888-33-5	5888335	3257	Reach_2140	2307	3.07	0.27	3	2.07	0.27		-6.3	-6.1	-7.5	0.0%	0.0%	0.0%
3-cyclohexylpropionic acid	211-861-9	701-97-3	701973	3557	Reach_1516	2308	4.49	0.54	3				-5.9	-6.1	-7.7	0.0%	0.0%	0.0%
N,N-dimethyl-3-oxobutyramide	218-059-8	2044-64-6	2044646	2265	Reach_1750	2309	6.19	0.52	3	5.19	0.52		-5.5	-6.1	-7.7	0.0%	0.0%	0.0%
phenyl acetate	204-575-0	122-79-2	122792	382	Reach_1035	2310	4.80		1				-6.3	-6.1	-7.2	0.0%	0.0%	0.0%
heptan-2-ol	201-947-4	89-87-2	89872	3988	Reach_354	2311	4.13		1				-6.3	-6.1	-7.2	0.0%	0.0%	0.0%
hexahydro-4-methylphthalic anhydride	243-072-0	19438-60-9	19438609	2232	Reach_2480	2312	5.34	0.29	3	4.34	0.29		-6.3	-6.1	-7.6	0.0%	0.0%	0.0%
800-696-3	800-696-3	78605-96-6	78605966	3752	Reach_5047	2313	3.22	0.18	3	2.20	0.49		-6.3	-6.1	-7.4	0.0%	0.0%	0.0%
1,1'-(methylimino)dipropan-2-ol	224-536-1	4402-30-6	4402306	2919	Reach_2032	2314	5.44	0.47	3	4.39	0.81		-5.4	-6.1	-7.7	0.0%	0.0%	0.0%
diethyl 1,2-cyclopentanedicarboxylate	213-107-4	924-50-5	924505	4034	Reach_1594	2315	5.62		1				-6.3	-6.1	-7.6	0.0%	0.0%	0.0%
4-[(morpholinothio)thioxomethyl]morpholine	205-439-3	140-89-6	140896	1195	Reach_1152	2316	4.57	0.84	5	4.45	0.85		-5.2	-6.1	-7.8	0.0%	0.0%	0.0%
sodium p-(3-amino-4-methylbenzamido)benzenesulphonate	201-899-4	89-33-8	89338	3971	Reach_340	2317	5.62		1				-5.8	-6.1	-7.4	0.0%	0.0%	0.0%
methyl (R)-amino(4-hydroxyphenyl)acetate	202-870-9	100-61-8	100618	133	Reach_564	2318	4.25	1.17	11	3.25	0.73	33	-5.3	-6.1	-7.6	0.0%	0.0%	0.0%
mucochloric acid	201-752-4	87-56-9	87569	3935	Reach_310	2319	3.93	1.20	3				-5.4	-6.1	-7.7	0.0%	0.0%	0.0%
2,2-Dichloro-1-(3-methyl-2,3-dihydro-4H-1,4-benzoxazin-4-yl)eth	202-548-8	96-97-9	96979	4158	Reach_473	2320	4.62	0.71	3	3.62	0.71		-6.0	-6.1	-7.5	0.0%	0.0%	0.0%
bis[2-[2-(2-butoxyethoxy)ethoxy]ethyl] adipate	265-807-4	65520-46-9	65520469	3455	Reach_2874	2321	4.76	0.35	3	3.76	0.35		-5.5	-6.1	-7.6	0.0%	0.0%	0.0%
N,N,N',N'-tetramethyltrimethylenediamine	203-818-8	110-95-2	110952	1533	Reach_839	2322	4.26	0.64	3	3.51	1.15		-6.3	-6.1	-7.3	0.0%	0.0%	0.0%
oxiniacic acid	216-676-7	1638-86-4	1638864	2090	Reach_1702	2323	5.50		1				-5.2	-6.1	-7.8	0.0%	0.0%	0.0%
hexadecyl acrylate	236-492-0	13402-02-3	13402023	1875	Reach_2334	2324	5.15	0.26	3	4.56	0.15		-6.0	-6.1	-7.5	0.0%	0.0%	0.0%
propylphosphonic dichloride	202-685-3	98-60-2	98602	4189	Reach_515	2325	4.25	0.52	3				-6.3	-6.1	-7.3	0.0%	0.0%	0.0%
(+)-L-arginine hydrochloride	206-200-6	307-35-7	307357	2611	Reach_1232	2326	3.21	0.33	3				-5.8	-6.1	-7.4	0.0%	0.0%	0.0%
1,3-di-o-tolylguanidine	202-577-6	97-39-2	97392	4164	Reach_478	2327	3.97	0.22	3	3.10	0.22		-6.0	-6.1	-7.6	0.0%	0.0%	0.0%
OO-tert-butyl O-(2-ethylhexyl) peroxycarbonate	252-029-5	34443-12-4	34443124	2706	Reach_2678	2328	2.39		1				-6.3	-6.1	-7.5	0.0%	0.0%	0.0%
(R)-1-hydroxy-1-phenylacetone	210-676-0	621-29-4	621294	3362	Reach_1442	2329	4.01	1.40	3	3.01	1.40		-5.6	-6.1	-7.7	0.0%	0.0%	0.0%
3-hydroxy-2'-methoxy-2-naphthanilide	205-206-6	135-62-6	135626	1894	Reach_1133	2330	3.40		1				-5.5	-6.1	-7.5	0.0%	0.0%	0.0%
3-(p-tert-butylphenyl)-2-methylpropanol	223-786-9	4073-98-7	4073987	2864	Reach_2010	2331	3.90	1.63	3	3.02	1.70		-6.2	-6.1	-7.5	0.0%	0.0%	0.0%
valeronitrile	203-781-8	110-59-8	110598	1523	Reach_818	2332	5.90		1				-6.3	-6.1	-7.1	0.0%	0.0%	0.0%
O,O,O-tris(4-nitrophenyl) thiophosphate	222-314-9	3423-25-4	3423254	2696	Reach_1957	2333	4.05	0.78	3				-6.1	-6.1	-7.5	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [ ]	Z(Cwfresh) [ ]	Z(Cwcoast) [ ]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
diethyl carbonate	203-311-1	105-58-8	105588	179	Reach_644	2334	5.09	0.75	6	4.70	0.75		-6.3	-6.1	-7.3	0.0%	0.0%	0.0%
isopentyl acetate	204-662-3	123-92-2	123922	398	Reach_1061	2335	5.00	0.38	3	4.00	0.38		-6.3	-6.1	-7.4	0.0%	0.0%	0.0%
chloro(methyl)silane	213-600-4	993-00-0	993000	4201	Reach_1626	2336	5.50	0.25	3	4.51	0.26		-6.5	-6.1	-8.2	0.0%	0.0%	0.0%
methyl benzoate	202-259-7	93-58-3	93583	4073	Reach_403	2337	4.85	0.66	3	3.85	0.66		-6.3	-6.1	-7.4	0.0%	0.0%	0.0%
2-ethylanthraquinone	201-535-4	84-51-5	84515	3867	Reach_285	2338	2.44		2				-6.3	-6.1	-7.5	0.0%	0.0%	0.0%
ethyldiisopropylamine	230-392-0	7087-68-5	7087685	814	Reach_2225	2339	4.95	0.70	16	3.95	0.70		-6.3	-6.1	-7.3	0.0%	0.0%	0.0%
601-327-7	605-152-7	15854-73-6	15854736	2063	Reach_4169	2340	4.24	0.17	3				-6.3	-6.1	-7.5	0.0%	0.0%	0.0%
Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]l	237-331-7	13749-61-6	13749616	1909	Reach_2348	2341	5.55	0.13	3	4.55	0.13		-5.8	-6.1	-6.7	0.0%	0.0%	0.0%
Disodium hydroxy(sulfonato)acetate	608-408-6	29736-24-1	29736241	5824	Reach_4275	2342	5.49		1				-5.8	-6.1	-7.4	0.0%	0.0%	0.0%
3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-indene	224-778-8	4488-57-7	4488577	2933	Reach_2040	2343	4.04	0.47	3	3.04	0.47		-6.3	-6.1	-7.5	0.0%	0.0%	0.0%
1,6-dichlorohexane	264-840-1	64354-92-3	64354923	3434	Reach_2865	2344	3.60	0.22	3	2.60	0.22		-6.3	-6.1	-7.4	0.0%	0.0%	0.0%
N-isopropylmethacrylamide	290-824-9	90268-24-9	90268249	3996	Reach_2992	2345	5.26	1.21	3	4.26	1.21		-6.3	-6.1	-7.6	0.0%	0.0%	0.0%
oxydiethylene dibenzoate	204-407-6	120-55-8	120558	1714	Reach_997	2346	3.76	0.24	3	2.45	0.51		-6.3	-6.1	-7.6	0.0%	0.0%	0.0%
(1R)-1-[(4R,4aR,8aS)-2,6-bis(4-chlorophenyl)tetrahydro[1,3]dioxi	200-541-4	62-55-5	62555	766	Reach_65	2347	4.64	0.69	3	3.64	0.69		-5.4	-6.1	-7.0	0.0%	0.0%	0.0%
2,2-dichloro-1,1,1-trifluoroethane	206-190-3	306-83-2	306832	2607	Reach_1231	2348	4.63	0.32	3	3.63	0.32		-6.5	-6.1	-8.3	0.0%	0.0%	0.0%
1-phenylethyl hydroperoxide	254-639-7	39811-17-1	39811171	2849	Reach_2728	2349	3.70	0.50	3				-6.3	-6.1	-7.4	0.0%	0.0%	0.0%
3-[(2-hydroxyethyl)amino]propionamide	248-211-9	27076-30-8	27076308	2494	Reach_2597	2350	5.36	1.10	3				-5.3	-6.1	-7.8	0.0%	0.0%	0.0%
tripotassium propylsilanetriolate	201-919-1	89-57-6	89576	3980	Reach_345	2351	4.69	0.54	3	3.69	0.54		-5.8	-6.1	-7.4	0.0%	0.0%	0.0%
1,1'-[oxybis(ethyleneoxy)]diethylene	201-708-4	86-92-0	86920	3913	Reach_305	2352	1.82	2.86	3				-6.3	-6.1	-7.3	0.0%	0.0%	0.0%
3-methyl-1-p-tolyl-5-pyrazolone	240-241-0	16088-62-3	16088623	498	Reach_2411	2353	4.86	0.38	3				-5.7	-6.1	-7.6	0.0%	0.0%	0.0%
2-[2-(3-aminopropoxy)ethoxy]ethanol	610-513-7	502421-44-5	502421445	2998	Reach_4331	2354	4.28	0.47	3				-5.3	-6.1	-7.8	0.0%	0.0%	0.0%
608-271-2	608-271-2	28861-00-9	28861009	2547	Reach_4268	2355	4.54	1.22	3				-5.2	-6.1	-7.8	0.0%	0.0%	0.0%
3,5,5-trimethylhexanoyl chloride	253-168-4	36727-29-4	36727294	2775	Reach_2703	2356	4.27	0.95	3	3.97	0.63		-6.3	-6.1	-8.5	0.0%	0.0%	0.0%
1,3-benzodioxolane	205-992-0	274-09-9	274099	2504	Reach_1218	2357	4.63	0.82	3				-6.3	-6.1	-7.6	0.0%	0.0%	0.0%
N-[[(4-methylphenyl)sulfonyl]methyl]formamide	607-301-1	23996-53-4	23996534	2364	Reach_4236	2358	3.91	1.28	3				-5.3	-6.1	-7.9	0.0%	0.0%	0.0%
2-ethylhexyl methacrylate	211-708-6	688-84-6	688846	3529	Reach_1504	2359	4.02	1.12	3	2.80	1.23		-6.3	-6.1	-7.8	0.0%	0.0%	0.0%
N-ethyl-N-[2-[1-(2-methylpropoxy)ethoxy]ethyl]-4-(phenylazo)a	204-129-5	116-16-5	116165	1647	Reach_953	2360	3.86	0.28	3				-5.6	-6.1	-7.7	0.0%	0.0%	0.0%
3-[(2-Ammonio-4,5-dimethoxyphenyl)diazenyl]-4-methoxybenze	226-323-9	5351-04-2	5351042	1274	Reach_2102	2361	4.11	0.83	3				-5.2	-6.1	-7.8	0.0%	0.0%	0.0%
1-methylpiperidine	230-262-3	6994-25-8	6994258	3553	Reach_2218	2362	3.94	0.08	3				-6.3	-6.1	-7.2	0.0%	0.0%	0.0%
N-[3-(dimethylamino)propyl]formamide	227-652-0	5922-69-0	5922690	3269	Reach_2144	2363	3.93	0.53	3				-5.4	-6.1	-7.8	0.0%	0.0%	0.0%
[1,3-phenylenebis(1-methylethylidene)]bis[tert-butyl] peroxide	218-664-7	2212-81-9	2212819	2320	Reach_1772	2364	5.88		1				-6.1	-6.1	-7.1	0.0%	0.0%	0.0%
octane-1,2-diol	214-254-7	1117-86-8	1117868	1557	Reach_1651	2365	4.54	0.70	3	3.71	0.73		-6.2	-6.1	-7.6	0.0%	0.0%	0.0%
diisopropyl 3,3'-[(2,5-dichloro-1,4-phenylene)bis[iminocarbonyl(	262-062-7	60113-43-1	60113431	3305	Reach_2844	2366	3.73		1				-6.3	-6.1	-5.2	0.0%	0.0%	0.0%
1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthyl)ethan-	216-133-4	1506-02-1	1506021	2011	Reach_1688	2367	2.92	0.39	3	1.92	0.39		-6.3	-6.1	-7.1	0.0%	0.0%	0.0%
1-[2-amino-1-(4-methoxyphenyl)ethyl]cyclohexanol hydrochloric	603-392-7	130198-05-9	130198059	5658	Reach_4118	2368							-5.8	-6.1	-7.5	0.0%	0.0%	0.0%
bis(1,2,2,6,6-pentamethyl-4-piperidyl) [[3,5-bis(1,1-dimethylethy	264-513-3	63843-89-0	63843890	3419	Reach_2863	2369	4.81		2	0.55			-6.1	-6.1	-6.5	0.0%	0.0%	0.0%
2-amino-2-ethylpropanediol	204-101-2	115-70-8	115708	1638	Reach_943	2370	5.55	0.35	3	4.43	0.41		-5.4	-6.1	-7.7	0.0%	0.0%	0.0%
palmitoyl chloride	203-996-7	112-67-4	112674	1597	Reach_918	2371	3.64	1.10	3	2.64	1.10		-6.3	-6.1	-8.3	0.0%	0.0%	0.0%
1,2,3,6-tetrahydromethyl-3,6-methanophthalic anhydride	246-644-8	25134-21-8	25134218	2417	Reach_2559	2372	5.56		1	4.45			-6.3	-6.1	-7.7	0.0%	0.0%	0.0%
Methyl 1,3,3-trimethyl-2-methylidene-2,3-dihydro-1H-indole-5-c	700-542-4	917392-54-2	917392542	4020	Reach_4929	2373	3.86	0.65	3				-6.3	-6.1	-7.5	0.0%	0.0%	0.0%
ethanesulphonyl chloride	223-684-4	4023-34-1	4023341	2855	Reach_2006	2374	4.76	0.64	3				-6.3	-6.1	-7.5	0.0%	0.0%	0.0%
undecan-1-ol	203-970-5	112-42-5	112425	329	Reach_906	2375	3.21	0.28	5	2.21	0.28		-6.3	-6.1	-7.4	0.0%	0.0%	0.0%
bis(2-ethoxyethyl) ether	230-625-6	7226-23-5	7226235	3600	Reach_2231	2376	5.71		2				-6.3	-6.1	-7.7	0.0%	0.0%	0.0%
3,3'-dimethoxybiphenyl-4,4'-ylenediammonium dichloride	235-464-5	12236-64-5	12236645	1748	Reach_2308	2377	5.01	1.08	3	4.01	1.08		-5.9	-6.1	-7.5	0.0%	0.0%	0.0%
tetrahydro-1,3-dimethyl-1H-pyrimidin-2-one	221-659-2	3179-63-3	3179633	2636	Reach_1928	2378	5.01	0.27	3	4.22	0.31		-6.3	-6.1	-7.8	0.0%	0.0%	0.0%
hydroxyprogesterone acetate	206-119-6	302-23-8	302238	2588	Reach_1229	2379	3.75	0.59	3				-5.6	-6.1	-7.6	0.0%	0.0%	0.0%
7-methyl-3-methyleneocta-1,6-diene	204-622-5	123-35-3	123353	390	Reach_1046	2380	4.89	0.70	3	3.89	0.70		-6.3	-6.1	-8.3	0.0%	0.0%	0.0%
2-chloro-4-nitrotoluene	211-631-8	676-83-5	676835	3499	Reach_1496	2381	4.53	0.77	3				-6.3	-6.1	-7.1	0.0%	0.0%	0.0%
7-acetamido-4-hydroxy-3-[[4-[[2-(sulphooxy)ethyl]sulphonyl]phe	287-574-8	85536-87-4	85536874	6061	Reach_2986	2382	5.33	0.92	3	4.33	0.92		-5.9	-6.1	-7.5	0.0%	0.0%	0.0%
Ethyl 3-oxo-3-(2,3,4,5-tetrafluorophenyl)propanoate	226-984-3	5586-73-2	5586732	3181	Reach_2128	2383	3.33	0.61	3				-6.3	-6.1	-7.6	0.0%	0.0%	0.0%
dioctyl ether	211-112-6	629-82-3	629823	3392	Reach_1471	2384	5.53	0.75	3	4.53	0.75		-6.2	-6.1	-8.3	0.0%	0.0%	0.0%
1,1,1,2,3,3,3-heptafluoropropane	207-079-2	431-89-0	431890	2907	Reach_1271	2385	5.12	0.59	3	4.12	0.59		-6.4	-6.1	-8.3	0.0%	0.0%	0.0%
[[p-(2-methoxyethyl)phenoxy]methyl]oxirane	221-877-8	3266-23-7	3266237	2657	Reach_1938	2386	5.26	0.32	3	4.26	0.32		-6.3	-6.1	-7.7	0.0%	0.0%	0.0%
6-tert-butyl-2,4-xylenol	217-533-1	1879-09-0	1879090	2209	Reach_1730	2387	3.55	0.15	3	2.55	0.15		-6.3	-6.1	-7.4	0.0%	0.0%	0.0%
bis(2-butoxyethyl) ether	204-001-9	112-73-2	112732	1600	Reach_921	2388	4.86	0.40	3	4.12	0.48		-6.3	-6.1	-7.7	0.0%	0.0%	0.0%
1,1,3,3-tetramethyldisiloxane	221-906-4	3277-26-7	3277267	2662	Reach_1940	2389	5.68	0.32	3	4.39	0.43		-6.5	-6.1	-8.2	0.0%	0.0%	0.0%
methyl 5-deoxy-2,3-O-isopropylidene-β-D-ribofuranoside	208-859-5	544-10-5	544105	3142	Reach_1352	2390	4.44		1				-6.3	-6.1	-7.5	0.0%	0.0%	0.0%
4-tert-butyltoluene	202-675-9	98-51-1	98511	1071	Reach_508	2391	3.50	0.70	16	2.92	0.70		-6.4	-6.1	-8.1	0.0%	0.0%	0.0%
tert-butyl methacrylate	209-548-7	585-07-9	585079	3248	Reach_1385	2392	5.50		1	3.42			-6.3	-6.1	-7.5	0.0%	0.0%	0.0%
Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]l	609-057-1	35052-92-7	35052927	5854	Reach_4287	2393							-5.9	-6.1	-7.7	0.0%	0.0%	0.0%
3,4,5,6,7,8,9,10,11,12,13,14-dodecahydro-2H-cyclododeca[b]pyr	251-090-5	32539-83-6	32539836	2655	Reach_2662	2394	2.20	0.71	3				-6.3	-6.1	-7.4	0.0%	0.0%	0.0%
diethyl fluoromalonate	216-490-6	1599-67-3	1599673	2070	Reach_1698	2395	-1.21	1.01	3				-6.3	-6.1	-7.5	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
isopropyl laurate	233-560-1	10233-13-3	10233133	1339	Reach_2284	2396	3.88	1.89	3	2.88	1.89		-6.3	-6.1	-8.2	0.0%	0.0%	0.0%
4-{2-[2-(2-hydroxybenzylidene)hydrazino]-2-oxoethyl}-4-methyl	700-714-9	1254469-57-2	1254469572	5643	Reach_4977	2397	4.67	0.10	3	3.74	0.17		-5.9	-6.1	-7.5	0.0%	0.0%	0.0%
isopropyl chloroformate	203-563-2	108-23-6	108236	1479	Reach_736	2398	4.64	0.51	3				-6.4	-6.1	-7.9	0.0%	0.0%	0.0%
1,1'-(methylenedi-p-phenylene)bismaleimide	238-969-9	14901-07-6	14901076	477	Reach_2373	2399	3.48	0.20	3	2.48	0.20		-5.3	-6.1	-7.7	0.0%	0.0%	0.0%
4-chloro-α,α,α-trifluoro-3-nitrotoluene	204-451-6	121-17-5	121175	1723	Reach_1008	2400	3.49		2				-6.4	-6.1	-7.7	0.0%	0.0%	0.0%
3-methoxypropylamine	226-241-3	5332-73-0	5332730	3095	Reach_2097	2401	4.72	0.32	3	3.86	0.78		-6.3	-6.1	-7.6	0.0%	0.0%	0.0%
tetramethyl orthosilicate	211-656-4	681-84-5	681845	3508	Reach_1497	2402	5.72	0.60	3	4.72	0.60		-6.3	-6.1	-7.4	0.0%	0.0%	0.0%
N-(4-chloro-2,5-dimethoxyphenyl)-2-[[2,5-dimethoxy-4-[(phenyl	235-427-3	12225-18-2	12225182	1745	Reach_2305	2403	4.43	0.88	3	3.43	0.88		-5.7	-6.1	-7.8	0.0%	0.0%	0.0%
cholesterol	200-353-2	57-88-5	57885	3240	Reach_44	2404	0.74	0.48	3				-5.9	-6.1	-6.8	0.0%	0.0%	0.0%
6,15-dihydroanthrazine-5,9,14,18-tetrone	201-375-5	81-77-6	81776	940	Reach_277	2405	4.66		1				-5.5	-6.1	-6.6	0.0%	0.0%	0.0%
isobutyryl chloride	201-194-1	79-30-1	79301	3770	Reach_238	2406	4.12	1.03	3	4.20	0.87		-6.4	-6.1	-7.9	0.0%	0.0%	0.0%
3,4-dimethoxyphenylacetonitrile	619-811-1	287930-71-6	287930716	5819	Reach_4547	2407							-6.2	-6.1	-7.8	0.0%	0.0%	0.0%
3,3'-[(2,5-dichloro-p-phenylene)bis[imino(1-acetyl-2-oxoethylene	219-292-8	2403-89-6	2403896	2369	Reach_1798	2408	4.11	0.80	3	3.11	0.80		-6.0	-6.1	-6.9	0.0%	0.0%	0.0%
heptanoyl chloride	219-775-3	2528-61-2	2528612	2428	Reach_1831	2409	4.32	1.04	4	3.32	1.04		-6.4	-6.1	-8.2	0.0%	0.0%	0.0%
dodecanenitrile	219-440-1	2437-25-4	2437254	559	Reach_1810	2410	2.88		1				-6.4	-6.1	-7.3	0.0%	0.0%	0.0%
2,2-difluoro-1,3-benzodioxole	210-565-7	618-83-7	618837	3357	Reach_1439	2411	5.40		2				-6.4	-6.1	-7.5	0.0%	0.0%	0.0%
605-350-3	605-350-3	16397-70-9	16397709	2091	Reach_4172	2412	4.04		1				-6.3	-6.1	-7.6	0.0%	0.0%	0.0%
valeryl chloride	211-330-1	638-29-9	638299	3418	Reach_1477	2413	4.70	0.81	4	3.98	0.63		-6.4	-6.1	-8.0	0.0%	0.0%	0.0%
decyldimethylamine	214-302-7	1120-24-7	1120247	1568	Reach_1656	2414	2.22	0.78	3	1.23	0.83		-6.4	-6.1	-8.2	0.0%	0.0%	0.0%
3'-chloropropiophenone	252-242-3	34841-35-5	34841355	2716	Reach_2683	2415	5.27		2				-6.4	-6.1	-7.4	0.0%	0.0%	0.0%
α,α,α',α'-tetramethyl-m-xylene-α,α'-diol	217-886-1	1999-85-5	1999855	2247	Reach_1742	2416	5.47	0.73	3	4.47	0.73		-5.8	-6.1	-7.7	0.0%	0.0%	0.0%
2-bromo-2-methylpropionyl bromide	213-339-6	938-18-1	938181	4085	Reach_1612	2417	3.66	0.23	3				-6.4	-6.1	-8.0	0.0%	0.0%	0.0%
Propanenitrile, 3-[[3-(tridecyloxy)propyl]amino]-, branched	203-810-4	110-87-2	110872	1532	Reach_834	2418	4.94		2				-6.1	-6.1	-7.8	0.0%	0.0%	0.0%
cyclohexyl methacrylate	202-943-5	101-43-9	101439	1322	Reach_578	2419	4.80	0.87	3	3.80	0.87		-6.4	-6.1	-7.5	0.0%	0.0%	0.0%
methyl 3-aminocrotonate	210-249-9	611-07-4	611074	3325	Reach_1418	2420	3.96		1				-6.3	-6.1	-7.5	0.0%	0.0%	0.0%
620-460-1	620-460-1	34494-24-1	34494241	2708	Reach_4570	2421	4.63	1.23	3				-5.3	-6.1	-7.8	0.0%	0.0%	0.0%
methylcyclohexane	203-624-3	108-87-2	108872	246	Reach_759	2422	4.19	1.44	8	1.44	0.70		-6.4	-6.1	-8.4	0.0%	0.0%	0.0%
3-ethyloxetane-3-methanol	221-254-0	3047-32-3	3047323	2598	Reach_1904	2423	6.78	0.19	3	6.01	0.25		-6.3	-6.1	-7.7	0.0%	0.0%	0.0%
diethyl phosphonate	212-091-6	762-04-9	762049	3705	Reach_1534	2424	5.32	0.41	3	4.32	0.41		-6.3	-6.1	-7.5	0.0%	0.0%	0.0%
606-753-7	620-464-3	1003859-14-0	1003859140	1303	Reach_4571	2425	5.00		1				-5.3	-6.1	-7.9	0.0%	0.0%	0.0%
methylurea	208-031-3	506-30-9	506309	3012	Reach_1310	2426	3.84	0.56	3	2.84	0.56		-6.2	-6.1	-7.7	0.0%	0.0%	0.0%
Salt of (8α,9R)-cinchonan-9-ol and [(R)-[(1S)-2-methyl-1-(1-oxopr	204-118-5	115-96-8	115968	10	Reach_948	2427	5.21	0.81	13	4.21	0.81	13	-5.9	-6.1	-7.5	0.0%	0.0%	0.0%
cyclohexapentylose	233-007-4	10016-20-3	10016203	1295	Reach_2277	2428	5.39	0.42	3	4.39	0.42		-6.0	-6.1	-7.5	0.0%	0.0%	0.0%
octadecylamine	204-695-3	124-30-1	124301	1791	Reach_1076	2429	2.25	0.78	3	1.48	0.71		-6.2	-6.2	-8.0	0.0%	0.0%	0.0%
2,2-Difluoroethanamine	278-077-7	75128-73-3	75128733	3658	Reach_2945	2430	5.01	1.35	3				-6.3	-6.2	-7.4	0.0%	0.0%	0.0%
3-methylpentane-1,5-diol	235-837-2	13001-46-2	13001462	5654	Reach_2315	2431	4.59	0.69	3	4.08	0.53		-6.2	-6.2	-7.8	0.0%	0.0%	0.0%
1,3-dihydro-1,3-dioxo-2H-isoindole-2-hexanoic acid	224-675-8	4443-26-9	4443269	2925	Reach_2037	2432	5.82	0.67	3	4.82	0.67		-5.4	-6.2	-7.7	0.0%	0.0%	0.0%
trichloro(ethyl)silane	204-072-6	115-21-9	115219	1633	Reach_940	2433	5.55	0.29	3	4.55	0.29		-6.4	-6.2	-7.7	0.0%	0.0%	0.0%
2,4-dichloro-3-ethyl-6-aminophenol	214-406-2	1125-21-9	1125219	1591	Reach_1662	2434	5.50		1				-5.6	-6.2	-7.9	0.0%	0.0%	0.0%
thioacetamide	214-912-3	1210-35-1	1210351	1721	Reach_1674	2435	3.48	0.38	3				-5.7	-6.2	-6.9	0.0%	0.0%	0.0%
614-284-4	603-758-6	133647-88-8	133647888	5668	Reach_4128	2436	5.30	0.27	3	4.30	0.27		-6.4	-6.2	-7.8	0.0%	0.0%	0.0%
3-(4-tert-butylphenyl)propionaldehyde	242-016-2	18127-01-0	18127010	2166	Reach_2452	2437	3.33	0.18	3	2.33	0.18		-6.4	-6.2	-7.4	0.0%	0.0%	0.0%
3,9-dicyclohex-3-enyl-2,4,8,10-tetraoxaspiro[5.5]undecane	212-133-3	764-99-8	764998	3714	Reach_1538	2438	5.47	0.31	3	4.47	0.31		-6.0	-6.2	-7.6	0.0%	0.0%	0.0%
1,2-dibromo-1,1,2,3,3,3-hexafluoropropane	210-513-3	617-45-8	617458	3351	Reach_1434	2439	5.11		1				-6.4	-6.2	-8.4	0.0%	0.0%	0.0%
3-(m-tert-butylphenyl)-2-methylpropionaldehyde	206-939-4	402-31-3	402313	2854	Reach_1266	2440	3.36		1				-6.4	-6.2	-7.4	0.0%	0.0%	0.0%
4,4'-methylenedi-2,6-xylenol	226-378-9	5384-21-4	5384214	3112	Reach_2104	2441	2.54		2				-5.7	-6.2	-7.4	0.0%	0.0%	0.0%
butyronitrile	203-700-6	109-74-0	109740	1507	Reach_788	2442	5.23	0.42	3				-6.4	-6.2	-7.2	0.0%	0.0%	0.0%
N,N-diethylhydroxylamine	223-055-4	3710-84-7	3710847	2791	Reach_1987	2443	4.81	0.71	3	3.81	0.71		-5.9	-6.2	-7.8	0.0%	0.0%	0.0%
3,4-dichloro-α,α,α-trifluorotoluene	248-885-4	28178-42-9	28178429	2524	Reach_2614	2444							-6.4	-6.2	-8.3	0.0%	0.0%	0.0%
2-bromopropane	203-558-5	108-18-9	108189	231	Reach_732	2445	5.14	0.59	19	3.76	0.70	16	-6.4	-6.2	-8.4	0.0%	0.0%	0.0%
prasterone	200-175-5	53-43-0	53430	3101	Reach_20	2446	3.37		2				-5.6	-6.2	-7.6	0.0%	0.0%	0.0%
undecane	214-300-6	1120-21-4	1120214	1567	Reach_1655	2447	5.93	2.41	3	4.93	2.41		-6.4	-6.2	-8.5	0.0%	0.0%	0.0%
2-methylbutyronitrile	700-143-5	959624-24-9	959624249	4139	Reach_4779	2448	4.00	0.59	3				-6.4	-6.2	-7.4	0.0%	0.0%	0.0%
trichloro(2,4,4-trimethylpentyl)silane	613-073-4	6271-80-3	6271803	3376	Reach_4379	2449	2.89		1				-6.4	-6.2	-7.9	0.0%	0.0%	0.0%
1,4-bis[(2,6-diethyl-4-methylphenyl)amino]anthraquinone	251-178-3	32724-62-2	32724622	2660	Reach_2665	2450	-0.96	0.87	3				-6.4	-6.2	-6.5	0.0%	0.0%	0.0%
Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol	272-469-1	68855-18-5	68855185	3527	Reach_2910	2451	1.68	0.57	3	0.68	0.57		-6.3	-6.2	-7.7	0.0%	0.0%	0.0%
6-[[(4-methylphenyl)sulphonyl]amino]hexanoic acid	278-934-5	78521-39-8	78521398	3751	Reach_2954	2452	6.03	0.49	3	5.03	0.49		-5.6	-6.2	-7.8	0.0%	0.0%	0.0%
Ethyl 1-[(2'-cyanobiphenyl-4-yl)methyl]-4-(2-hydroxypropan-2-yl	201-377-6	81-81-2	81812	942	Reach_278	2453	4.45	1.19	6	3.45	1.19		-5.8	-6.2	-7.8	0.0%	0.0%	0.0%
1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-8-iodooctane	606-722-8	211915-06-9	211915069	2286	Reach_4213	2454	2.47	0.20	3				-6.3	-6.2	-8.3	0.0%	0.0%	0.0%
1,3-dimethylimidazolidin-2-one	201-304-8	80-73-9	80739	3797	Reach_269	2455	5.25	0.27	3	4.25	0.27		-6.3	-6.2	-7.9	0.0%	0.0%	0.0%
methyl 4-[[(2,5-dichlorophenyl)amino]carbonyl]-2-[[2-hydroxy-3	263-272-1	61847-48-1	61847481	3356	Reach_2852	2456	5.04	1.10	3	4.04	1.10		-5.8	-6.2	-6.8	0.0%	0.0%	0.0%
2-Chloro-2-methylpropanoyl chloride	202-188-1	92-77-3	92773	4049	Reach_392	2457	3.22	0.13	3				-6.5	-6.2	-7.9	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
piperonal	204-409-7	120-57-0	120570	1715	Reach_998	2458	4.11	0.68	3	3.04	0.62		-6.4	-6.2	-7.7	0.0%	0.0%	0.0%
2,2-dimethyl-1,3-propanediyl dioctanoate	250-575-9	31335-74-7	31335747	2625	Reach_2654	2459	1.68	0.57	3	0.68	0.57		-6.1	-6.2	-7.3	0.0%	0.0%	0.0%
Dimethyl((2-oxocyclohexyl)methyl)ammonium chloride	617-143-5	80675-49-6	80675496	3796	Reach_4446	2460	3.27	0.70	3				-5.9	-6.2	-7.5	0.0%	0.0%	0.0%
o-phenetidine	202-356-4	94-70-2	94702	4109	Reach_417	2461	3.82	0.69	3				-5.7	-6.2	-7.8	0.0%	0.0%	0.0%
allyl methacrylate	202-473-0	96-05-9	96059	1043	Reach_449	2462	3.46	0.73	4	2.63	0.69		-6.4	-6.2	-7.6	0.0%	0.0%	0.0%
ethyl 2-bromobutyrate	208-574-6	533-68-6	533686	3099	Reach_1330	2463	4.31	1.21	3				-6.4	-6.2	-7.6	0.0%	0.0%	0.0%
isobutyl acrylate	203-417-8	106-63-8	106638	198	Reach_675	2464	3.57	0.41	5	2.87	0.46		-6.4	-6.2	-7.6	0.0%	0.0%	0.0%
2,2,4-trimethylpentane-1,3-diol	205-619-1	144-19-4	144194	1974	Reach_1194	2465	5.86	0.37	3	4.86	0.37		-6.1	-6.2	-7.7	0.0%	0.0%	0.0%
5-ethoxy-7-fluoro[1,2,4]triazolo[4,3-c]pyrimidine-3(2H)-thione	695-186-9	166524-68-1	166524681	2106	Reach_4688	2466							-5.4	-6.2	-7.8	0.0%	0.0%	0.0%
606-938-2	606-938-2	2212-11-5	2212115	1244	Reach_4226	2467							-6.4	-6.2	-7.4	0.0%	0.0%	0.0%
methyl (R)-aminophenylacetate	204-594-4	123-04-6	123046	1760	Reach_1037	2468	3.65	0.65	3	2.65	0.65		-5.4	-6.2	-7.8	0.0%	0.0%	0.0%
2,3-dichlorotoluene	256-636-6	50594-82-6	50594826	3011	Reach_2766	2469	2.99	0.11	3				-6.4	-6.2	-7.7	0.0%	0.0%	0.0%
(chloromethyl)triethoxysilane	239-311-3	15267-95-5	15267955	2025	Reach_2380	2470	5.63	0.51	3	4.63	0.51		-6.4	-6.2	-7.8	0.0%	0.0%	0.0%
methyl 2-amino-4-[[(2,5-dichlorophenyl)amino]carbonyl]benzoa	261-853-4	59673-82-4	59673824	3283	Reach_2839	2471	3.62	0.11	3				-5.8	-6.2	-7.9	0.0%	0.0%	0.0%
1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone	208-806-6	542-18-7	542187	687	Reach_1346	2472	3.60		1				-5.4	-6.2	-7.9	0.0%	0.0%	0.0%
1,2-dihydro-5-nitro-3H-1,2,4-triazol-3-one	213-254-4	932-64-9	932649	4066	Reach_1610	2473	5.85	0.67	3	4.85	0.67		-5.3	-6.2	-8.0	0.0%	0.0%	0.0%
3-chloropropyne	201-568-4	84-87-7	84877	3880	Reach_291	2474	4.84	0.32	3				-6.5	-6.2	-8.0	0.0%	0.0%	0.0%
acetone-dimethyl acetal	217-218-9	1779-49-3	1779493	5743	Reach_1719	2475	3.55		1				-6.4	-6.2	-7.7	0.0%	0.0%	0.0%
2,2-bis(bromomethyl)propane-1,3-diol	221-967-7	3296-90-0	3296900	2671	Reach_1943	2476	5.12	0.47	3	4.12	0.47		-5.6	-6.2	-7.8	0.0%	0.0%	0.0%
1-(dimethylamino)propan-2-ol	203-556-4	108-16-7	108167	1477	Reach_731	2477	4.99	0.14	3	4.32	0.55		-6.4	-6.2	-7.8	0.0%	0.0%	0.0%
6-[methyl(phenylsulphonyl)amino]hexanoic acid, compound wit	248-107-3	26919-50-6	26919506	5807	Reach_2596	2478	5.58	0.79	3	4.58	0.79		-5.9	-6.2	-7.5	0.0%	0.0%	0.0%
N-phenyl-N-[(trichloromethyl)thio]benzenesulphonamide	223-054-9	3710-30-3	3710303	2790	Reach_1986	2479	3.14	0.33	3	2.14	0.33		-6.0	-6.2	-7.7	0.0%	0.0%	0.0%
N-[3-(dimethoxymethylsilyl)propyl]ethylenediamine	221-336-6	3069-29-2	3069292	2608	Reach_1909	2480	4.62	0.96	3	3.62	0.96		-6.1	-6.2	-7.8	0.0%	0.0%	0.0%
4-(2,6,6-trimethylcyclohex-1-ene-1-yl)-but-3-ene-2-one	219-110-7	2362-14-3	2362143	2353	Reach_1785	2481	3.06	0.43	3	2.06	0.43		-6.4	-6.2	-7.2	0.0%	0.0%	0.0%
N,N'-diacetylhydrazine	221-576-1	3148-73-0	3148730	2627	Reach_1921	2482	6.06	0.98	3	5.06	0.98		-5.4	-6.2	-7.9	0.0%	0.0%	0.0%
2-chloropropane	200-858-8	75-29-6	75296	3664	Reach_137	2483	5.31	0.25	3	4.31	0.25		-6.5	-6.2	-8.4	0.0%	0.0%	0.0%
methyl 3-methyl-2-butenoate	937-695-3	1185167-55-8	1185167558	5618	Reach_5146	2484							-6.4	-6.2	-7.5	0.0%	0.0%	0.0%
29H,31H-phthalocyanine	237-335-9	13752-51-7	13752517	1911	Reach_2349	2485	3.76	0.43	3	2.76	0.43		-6.0	-6.2	-6.8	0.0%	0.0%	0.0%
α-bromotoluene	228-545-1	6291-85-6	6291856	3387	Reach_2162	2486	4.06	0.39	3				-6.4	-6.2	-7.6	0.0%	0.0%	0.0%
618-990-3	618-990-3	939961-06-5	939961065	6087	Reach_4506	2487							-5.9	-6.2	-7.6	0.0%	0.0%	0.0%
phosgene	202-452-6	95-79-4	95794	4135	Reach_442	2488	4.02		2				-6.7	-6.2	-8.4	0.0%	0.0%	0.0%
ethyl 3-amino-1H-pyrazole-4-carboxylate	200-362-1	58-08-2	58082	66	Reach_45	2489	4.59	1.55	5	1.29	1.05		-5.3	-6.2	-7.9	0.0%	0.0%	0.0%
isodecyl methacrylate	249-978-2	29964-84-9	29964849	2581	Reach_2640	2490	3.46	1.77	3	2.46	1.77		-6.4	-6.2	-7.9	0.0%	0.0%	0.0%
1-(vinyloxy)octadecane	609-335-2	3717-40-6	3717406	2792	Reach_4297	2491	4.68	0.35	3	3.68	0.35		-6.1	-6.2	-7.6	0.0%	0.0%	0.0%
3,3'-[butane-1,4-diylbis(oxy)]bispropanamine	201-832-9	88-45-9	88459	3957	Reach_324	2492	4.88	0.76	3	3.88	0.76		-5.4	-6.2	-7.9	0.0%	0.0%	0.0%
octyltrichlorosilane	226-112-1	5283-66-9	5283669	678	Reach_2093	2493	5.54	0.13	4	4.54	0.13		-6.4	-6.2	-7.3	0.0%	0.0%	0.0%
2,4,6-tri-tert-butylphenol	211-989-5	732-26-3	732263	829	Reach_1524	2494	1.78	0.84	4	0.78	0.84		-6.3	-6.2	-7.3	0.0%	0.0%	0.0%
611-869-6	700-691-5	473799-16-5	473799165	2965	Reach_4969	2495	1.07		3				-6.4	-6.2	-7.4	0.0%	0.0%	0.0%
4-amino-6-chlorobenzene-1,3-disulphonamide	204-463-1	121-30-2	121302	1724	Reach_1009	2496	5.92		2				-5.3	-6.2	-8.1	0.0%	0.0%	0.0%
dodecane	203-967-9	112-40-3	112403	1587	Reach_904	2497	5.93	2.47	3	4.93	2.47		-6.4	-6.2	-8.5	0.0%	0.0%	0.0%
2,4,6-trimethyl-2,4,6-tris(3,3,3-trifluoropropyl)cyclotrisiloxane	219-154-7	2374-14-3	2374143	2357	Reach_1790	2498	1.38	0.52	3				-6.3	-6.2	-7.2	0.0%	0.0%	0.0%
1-(allyloxy)-2-methyl-1-oxopropan-2-yl 2-chloro-5-[3-methyl-2,6-	603-837-5	134605-64-4	134605644	433	Reach_4131	2499	3.07	1.28	9	0.49	0.97		-5.8	-6.2	-7.4	0.0%	0.0%	0.0%
trans-crotonic acid	200-002-3	50-01-1	50011	2994	Reach_2	2500	5.13	0.91	3	4.13	0.91		-5.5	-6.2	-7.8	0.0%	0.0%	0.0%
chloroacetaldehyde	700-052-0	60046-50-6	60046506	3303	Reach_4741	2501	5.30	0.55	3				-6.5	-6.2	-7.5	0.0%	0.0%	0.0%
3,3'-sulphonyldianiline	209-967-5	599-61-1	599611	3298	Reach_1409	2502	4.00	0.81	3	3.00	0.81		-5.4	-6.2	-7.8	0.0%	0.0%	0.0%
4-tert-butylpyrocatechol	202-653-9	98-29-3	98293	4181	Reach_503	2503	3.04	0.64	3	1.91	0.65		-6.3	-6.2	-7.7	0.0%	0.0%	0.0%
1-nitropropane	203-544-9	108-03-2	108032	1475	Reach_726	2504	5.43	0.31	3	4.55	0.36		-6.4	-6.2	-7.8	0.0%	0.0%	0.0%
5-propyl-1,3-benzodioxole	202-344-9	94-58-6	94586	4105	Reach_415	2505							-6.4	-6.2	-7.5	0.0%	0.0%	0.0%
bis(2-ethylhexyl) succinate	202-165-6	92-54-6	92546	4039	Reach_386	2506	3.94	0.76	3				-6.2	-6.2	-7.3	0.0%	0.0%	0.0%
2-methylbutan-1-ol	204-050-6	114-49-8	114498	5612	Reach_934	2507							-6.4	-6.2	-7.5	0.0%	0.0%	0.0%
6-[(1-oxomethyloctyl)amino]hexanoic acid	203-702-7	109-76-2	109762	265	Reach_790	2508	5.46	0.67	4	4.30	0.61		-5.6	-6.2	-7.7	0.0%	0.0%	0.0%
4,4'-methylenedi-o-toluidine	223-342-4	3845-76-9	3845769	2822	Reach_1994	2509	4.69	0.74	3	3.69	0.74		-5.7	-6.2	-7.9	0.0%	0.0%	0.0%
bis(2-chloroethyl) 3,3'-[(2,5-dimethyl-p-phenylene)bis[iminocarb	261-819-9	59587-44-9	59587449	3281	Reach_2838	2510	1.97	0.43	3	5.00			-6.4	-6.2	-5.5	0.0%	0.0%	0.0%
1,1-difluoroethane	200-866-1	75-37-6	75376	3669	Reach_142	2511	5.15	0.36	3	4.15	0.36		-6.5	-6.2	-8.4	0.0%	0.0%	0.0%
11β,17,21-trihydroxypregna-1,4-diene-3,20-dione 21-methanesu	237-721-7	13940-94-8	13940948	1919	Reach_2352	2512	4.40		2				-5.4	-6.2	-7.9	0.0%	0.0%	0.0%
1-(2-hydroxyethyl)pyrrolidin-2-one	222-359-4	3445-11-2	3445112	1260	Reach_1962	2513	4.97	1.61	3				-5.2	-6.2	-7.8	0.0%	0.0%	0.0%
N,N-bis(3-aminopropyl)methylamine	277-873-1	74441-05-7	74441057	3635	Reach_2943	2514	4.17	1.01	3	3.17	1.01		-6.0	-6.2	-8.0	0.0%	0.0%	0.0%
dibutyl adipate	203-350-4	105-99-7	105997	184	Reach_653	2515	3.65	0.32	4	2.65	0.32		-6.4	-6.2	-7.5	0.0%	0.0%	0.0%
619-636-0	265-633-9	65212-76-2	65212762	5972	Reach_2870	2516	5.83		1				-5.7	-6.2	-7.8	0.0%	0.0%	0.0%
5-chloro-α,α,α-trifluoro-2-nitrotoluene	610-840-5	52449-76-0	52449760	3059	Reach_4336	2517	3.68	0.59	3	3.02	0.55		-6.4	-6.2	-7.5	0.0%	0.0%	0.0%
4-methyl-3-decen-5-ol	279-815-0	81782-77-6	81782776	3814	Reach_2961	2518	3.13	0.32	3	2.13	0.32		-6.4	-6.2	-7.6	0.0%	0.0%	0.0%
N,N''-(4-methyl-m-phenylene)bis[N',N'-dimethylurea]	241-523-6	17526-94-2	17526942	2141	Reach_2435	2519	3.86	2.17	3				-5.4	-6.2	-7.9	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
617-707-0	618-771-2	915725-52-9	915725529	6081	Reach_4499	2520							-5.4	-6.2	-7.9	0.0%	0.0%	0.0%
allylamine	203-463-9	107-11-9	107119	209	Reach_694	2521	4.41	0.54	28	3.64	0.70	12	-6.4	-6.2	-7.2	0.0%	0.0%	0.0%
(4-nonylphenoxy)acetic acid	221-486-2	3115-49-9	3115499	2619	Reach_1917	2522	3.90	0.58	3	3.18	0.66		-5.8	-6.2	-7.8	0.0%	0.0%	0.0%
2-[benzyl(2-hydroxyethyl)amino]-1-phenylethanol	203-994-6	112-64-1	112641	1596	Reach_917	2523	1.41	0.20	3				-5.4	-6.2	-7.9	0.0%	0.0%	0.0%
(R)-2,2,3-trimethylcyclopent-3-ene-1-acetaldehyde	224-815-8	4501-58-0	4501580	2937	Reach_2044	2524	4.01	0.19	3				-6.4	-6.2	-7.4	0.0%	0.0%	0.0%
2-methylbenzene-1,4-diyl bis{4-[4-(acryloyloxy)butoxy]benzoate	204-605-2	123-15-9	123159	385	Reach_1040	2525	4.47	0.26	4	3.47	0.26		-5.8	-6.2	-6.9	0.0%	0.0%	0.0%
N-(2-hydroxypropyl)oleamide	203-828-2	111-05-7	111057	1537	Reach_843	2526	1.47	0.26	3				-5.7	-6.2	-7.8	0.0%	0.0%	0.0%
610-513-7	211-745-8	693-21-0	693210	804	Reach_1505	2527	5.36	0.70	40	4.36	0.70		-5.6	-6.2	-7.8	0.0%	0.0%	0.0%
alpha,2-dichloro-6-fluorotoluene	201-813-5	88-23-3	88233	3953	Reach_321	2528	4.15	0.66	3				-6.5	-6.2	-7.6	0.0%	0.0%	0.0%
cyclooctapentylose	241-482-4	17465-86-0	17465860	6398	Reach_2434	2529	5.46	0.41	3	4.46	0.41		-6.0	-6.2	-7.6	0.0%	0.0%	0.0%
tetradecahydro-7-isopropyl-1,4a-dimethylphenanthren-1-metha	236-476-3	13393-93-6	13393936	1873	Reach_2333	2530	5.42	0.22	3	4.42	0.22		-6.1	-6.2	-7.3	0.0%	0.0%	0.0%
3,4-dimethoxyphenethylamine	614-070-0	674773-12-7	674773127	3492	Reach_4395	2531	3.96	0.31	3				-6.4	-6.2	-7.9	0.0%	0.0%	0.0%
N-(2-chlorobenzyl)-1-phenylpropan-2-amine hydrochloride (1:1)	695-069-2	1048649-80-4	1048649804	5594	Reach_4686	2532							-6.0	-6.2	-7.6	0.0%	0.0%	0.0%
1,1-dimethoxytrimethylamine	200-939-8	76-16-4	76164	3701	Reach_173	2533	4.72	0.18	3	3.72	0.18		-5.9	-6.2	-7.9	0.0%	0.0%	0.0%
isobutyric anhydride	202-603-6	97-72-3	97723	4171	Reach_485	2534	4.96	0.45	3	4.23	0.42		-6.4	-6.2	-7.6	0.0%	0.0%	0.0%
dichloro(chloromethyl)methylsilane	700-442-0	73573-88-3	73573883	3623	Reach_4900	2535	2.67	1.41	3				-6.5	-6.2	-8.1	0.0%	0.0%	0.0%
1,2,3,6-tetrahydro-3-methylphthalic anhydride	226-247-6	5333-84-6	5333846	3097	Reach_2099	2536	5.00	0.17	3	4.33	0.23		-6.4	-6.2	-7.8	0.0%	0.0%	0.0%
2,6-dimethylheptan-4-one	203-620-1	108-83-8	108838	1490	Reach_758	2537	4.63	0.24	3	3.60	0.38		-6.5	-6.2	-7.7	0.0%	0.0%	0.0%
1,4-bis(mesitylamino)anthraquinone	204-155-7	116-75-6	116756	1653	Reach_956	2538	3.64	1.49	3	2.64	1.49		-6.3	-6.2	-6.7	0.0%	0.0%	0.0%
610-555-6	619-405-4	99199-60-7	99199607	4199	Reach_4518	2539	5.06	0.33	3				-6.4	-6.2	-7.7	0.0%	0.0%	0.0%
methyl 4-tert-butylbenzoate	225-756-0	5056-17-7	5056177	3009	Reach_2074	2540	3.60	1.47	3				-6.5	-6.2	-7.4	0.0%	0.0%	0.0%
1,2-epoxycyclohexane	206-007-7	286-20-4	286204	2539	Reach_1221	2541	4.36	0.58	3				-6.5	-6.2	-7.4	0.0%	0.0%	0.0%
2,3-epoxypropan-1-ol	209-128-3	556-52-5	556525	703	Reach_1366	2542	5.44	0.88	4	4.44	0.88		-6.4	-6.2	-7.9	0.0%	0.0%	0.0%
phenyl chloroformate	205-498-5	141-75-3	141753	1941	Reach_1167	2543	4.33	1.12	3	4.17	1.10		-6.5	-6.2	-7.5	0.0%	0.0%	0.0%
dimethyl naphthalene-2,6-dicarboxylate	212-661-4	840-65-3	840653	3856	Reach_1565	2544	3.72	0.57	3				-6.5	-6.2	-7.8	0.0%	0.0%	0.0%
6-methyl-2-oxoperhydropyrimidin-4-ylurea	216-223-3	1530-32-1	1530321	2028	Reach_1689	2545	3.56	0.97	3	2.56	0.97		-5.4	-6.2	-7.9	0.0%	0.0%	0.0%
617-931-9	616-378-0	767340-03-4	767340034	3723	Reach_4436	2546							-6.5	-6.3	-7.3	0.0%	0.0%	0.0%
606-859-3	606-859-3	21890-10-8	21890108	2311	Reach_4221	2547	3.26	1.24	3				-6.4	-6.3	-7.8	0.0%	0.0%	0.0%
4,4'-[(6-chloro-1,3,5-triazine-2,4-diyl)diimino]bis[5-hydroxy-6-[[4	303-152-9	94158-79-9	94158799	6089	Reach_3007	2548							-6.0	-6.3	-7.6	0.0%	0.0%	0.0%
octamethylenediamine	206-764-3	373-44-4	373444	2796	Reach_1259	2549	4.74	0.57	3	3.74	0.57		-6.4	-6.3	-7.7	0.0%	0.0%	0.0%
tartaric anhydride dibenzoate	604-481-3	14559-13-8	14559138	1987	Reach_4156	2550	3.55	1.16	3				-5.2	-6.3	-7.9	0.0%	0.0%	0.0%
3-(isotridecyloxy)propylamine	256-881-9	50977-10-1	50977101	3024	Reach_2768	2551	2.39		2				-6.5	-6.3	-7.3	0.0%	0.0%	0.0%
bis(trimethoxysilylpropyl)amine	280-084-5	82985-35-1	82985351	3839	Reach_2964	2552	4.56	0.61	3	4.11	0.40		-5.7	-6.3	-8.1	0.0%	0.0%	0.0%
2-(2-hexyloxyethoxy)ethanol	203-988-3	112-59-4	112594	1593	Reach_914	2553	5.31	0.26	3	4.36	0.46		-5.7	-6.3	-7.9	0.0%	0.0%	0.0%
4,7-dihydro-2-isopropyl-1,3-dioxepin	700-842-5	1192015-20-5	1192015205	5620	Reach_5007	2554							-6.5	-6.3	-7.4	0.0%	0.0%	0.0%
undecanedioic acid	230-279-6	7005-47-2	7005472	3555	Reach_2219	2555	5.36		2				-5.7	-6.3	-7.9	0.0%	0.0%	0.0%
Tris[3-bromo-2,2-bis(bromomethyl)propyl] phosphate	606-254-4	19186-97-1	19186971	2226	Reach_4202	2556	1.37	1.30	3	3.51			-6.2	-6.3	-7.8	0.0%	0.0%	0.0%
hexyl acetate	205-572-7	142-92-7	142927	466	Reach_1186	2557	3.73	0.36	4	2.73	0.36		-6.5	-6.3	-7.6	0.0%	0.0%	0.0%
ethyl 2-bromo-2-methylpropionate	209-980-6	600-00-0	600000	3302	Reach_1411	2558	4.84		1				-6.5	-6.3	-7.9	0.0%	0.0%	0.0%
7-[(E)-(4-aminophenyl)diazenyl]naphthalene-1,3,5-trisulfonic aci	700-663-2	1035-69-4	1035694	1370	Reach_4962	2559	4.36	0.17	3				-5.3	-6.3	-7.9	0.0%	0.0%	0.0%
hexadecyl chloroformate	608-880-3	335153-21-4	335153214	2682	Reach_4284	2560	4.62		1				-6.3	-6.3	-8.2	0.0%	0.0%	0.0%
octadecyl isocyanate	204-019-7	112-96-9	112969	1614	Reach_932	2561	0.53	1.07	3				-6.2	-6.3	-7.5	0.0%	0.0%	0.0%
605-991-9	225-060-7	4635-87-4	4635874	2952	Reach_2051	2562	4.70		1				-5.9	-6.3	-7.9	0.0%	0.0%	0.0%
chlorodimethylvinylsilane	217-007-1	1719-58-0	1719580	2125	Reach_1712	2563	5.52	0.26	3	4.45	0.28		-6.5	-6.3	-8.6	0.0%	0.0%	0.0%
ethyl vinyl ether	203-718-4	109-92-2	109922	1512	Reach_797	2564	4.63	0.12	3	3.80	0.23		-6.6	-6.3	-8.5	0.0%	0.0%	0.0%
605-955-2	609-920-2	4137-56-8	4137568	2875	Reach_4316	2565	4.53	0.87	3				-5.8	-6.3	-7.9	0.0%	0.0%	0.0%
homosalate	204-260-8	118-56-9	118569	1673	Reach_965	2566	5.79		1				-6.1	-6.3	-7.5	0.0%	0.0%	0.0%
N-[3-(dimethylamino)propyl]-N,N',N'-trimethylpropane-1,3-diam	223-362-3	3855-32-1	3855321	2824	Reach_1996	2567	4.63	0.49	3	3.47	0.72		-6.4	-6.3	-8.0	0.0%	0.0%	0.0%
ethylene diformate	211-077-7	629-15-2	629152	3386	Reach_1465	2568	5.04	0.44	3	4.04	0.44		-6.4	-6.3	-7.9	0.0%	0.0%	0.0%
2-benzoyl-1,2,3,6,7,11b-hexahydro-4H-pyrazino[2,1-a]isoquinoli	600-478-6	1037197-98-0	1037197980	1379	Reach_4066	2569	2.43	0.69	3				-5.7	-6.3	-7.4	0.0%	0.0%	0.0%
vinyl laurate	620-166-3	32257-57-1	32257571	5843	Reach_4560	2570				5.09			-6.5	-6.3	-7.6	0.0%	0.0%	0.0%
4-methyloxazole-5-carboxamide	700-281-6	2897-00-9	2897009	2553	Reach_4840	2571	2.90	0.29	3				-5.3	-6.3	-7.9	0.0%	0.0%	0.0%
2,3-dichlorobuta-1,3-diene	216-721-0	1653-19-6	1653196	2099	Reach_1704	2572	3.31	0.19	3	2.59	0.40		-6.5	-6.3	-8.4	0.0%	0.0%	0.0%
800-884-5	800-884-5	1154308-86-7	1154308867	1636	Reach_5048	2573	4.58	0.54	3	3.58	0.54		-5.6	-6.3	-7.8	0.0%	0.0%	0.0%
(-)-pin-2(3)-ene	232-077-3	7785-26-4	7785264	887	Reach_2273	2574	3.39	0.97	3	2.39	0.97		-6.5	-6.3	-8.4	0.0%	0.0%	0.0%
diisopropyl succinate	213-110-0	924-88-9	924889	4037	Reach_1595	2575	4.42		1				-6.5	-6.3	-7.6	0.0%	0.0%	0.0%
decanal	203-957-4	112-31-2	112312	1581	Reach_897	2576	3.33	0.17	3	2.50	0.19		-6.5	-6.3	-7.8	0.0%	0.0%	0.0%
1,2-bis(2-methoxyethoxy)ethane	228-506-9	6284-40-8	6284408	770	Reach_2160	2577	6.17	0.65	4	5.17	0.65		-6.4	-6.3	-7.9	0.0%	0.0%	0.0%
N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2-met	257-515-0	51920-12-8	51920128	3049	Reach_2776	2578	4.17	1.05	3	3.17	1.05		-5.8	-6.3	-7.9	0.0%	0.0%	0.0%
2-Chloro-1,1-difluoroethane	201-984-6	90-31-3	90313	3997	Reach_363	2579	1.82	2.83	3				-6.7	-6.3	-8.5	0.0%	0.0%	0.0%
N,N'-hexane-1,6-diylbis(hexahydro-2-oxo-1H-azepine-1-carboxa	227-563-7	5888-87-9	5888879	3258	Reach_2141	2580	4.80	0.29	3	3.80	0.29		-5.6	-6.3	-7.8	0.0%	0.0%	0.0%
2-(Propylsulfanyl)pyrimidine-4,6(1H,5H)-dione	603-883-6	134931-01-4	134931014	1884	Reach_4132	2581	4.25	0.61	3				-5.4	-6.3	-7.9	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
1,1'-methylenebis[4-fluorobenzene]	207-274-2	457-68-1	457681	2945	Reach_1281	2582	3.13	0.12	3				-6.5	-6.3	-8.1	0.0%	0.0%	0.0%
clioquinol	200-431-6	59-50-7	59507	737	Reach_51	2583	3.79	0.73	42	2.65	0.73		-5.9	-6.3	-7.9	0.0%	0.0%	0.0%
1,6-dibromohexane	211-067-2	629-03-8	629038	3384	Reach_1463	2584	3.15		1				-6.5	-6.3	-7.8	0.0%	0.0%	0.0%
1-(3,4-dimethoxybicyclo[4.2.0]octa-1,3,5-trien-7-yl)methanamin	227-285-6	5763-44-0	5763440	3235	Reach_2134	2585	5.00		2				-6.0	-6.3	-7.9	0.0%	0.0%	0.0%
α,α,α-trifluoro-o-toluoyl chloride	206-233-6	312-94-7	312947	2624	Reach_1233	2586	3.48	0.99	3				-6.5	-6.3	-7.7	0.0%	0.0%	0.0%
1-[(2-chloro-4-nitrophenyl)azo]-2-naphthol	220-562-2	2814-77-9	2814779	2523	Reach_1872	2587	2.90	0.94	3				-5.9	-6.3	-7.2	0.0%	0.0%	0.0%
dibutyl fumarate	203-327-9	105-75-9	105759	182	Reach_649	2588	2.67	0.37	8	1.67	0.37		-6.5	-6.3	-7.6	0.0%	0.0%	0.0%
octadecane	211-659-0	682-01-9	682019	3509	Reach_1498	2589	5.19	0.93	3	4.19	0.93		-6.2	-6.3	-7.5	0.0%	0.0%	0.0%
hexadecyltrimethoxysilane	240-464-3	16415-12-6	16415126	2092	Reach_2419	2590	5.49	1.76	3	4.49	1.76		-6.3	-6.3	-7.4	0.0%	0.0%	0.0%
dodecan-5-olide	700-306-0	383412-05-3	383412053	2821	Reach_4852	2591	3.77	0.86	3				-6.5	-6.3	-7.5	0.0%	0.0%	0.0%
docosanamide	221-304-1	3061-75-4	3061754	2604	Reach_1908	2592	2.52	0.28	3	1.52	0.28		-6.1	-6.3	-7.0	0.0%	0.0%	0.0%
619-635-5	619-635-5	12567-73-6	12567736	5644	Reach_4533	2593							-6.0	-6.3	-7.6	0.0%	0.0%	0.0%
N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-2-[(4-nitrophenyl)az	249-955-7	29920-31-8	29920318	2579	Reach_2638	2594	4.17	1.01	3	3.17	1.01		-5.6	-6.3	-8.0	0.0%	0.0%	0.0%
6-(isononanoylamino)hexanoic acid, compound with 2,2',2''-nitri	203-842-9	111-18-2	111182	1540	Reach_847	2595	4.51	0.48	3	3.51	0.48		-5.7	-6.3	-7.8	0.0%	0.0%	0.0%
2-nitro-p-anisidine	202-547-2	96-96-8	96968	4157	Reach_472	2596	3.81	1.16	3	2.81	1.16		-5.7	-6.3	-8.0	0.0%	0.0%	0.0%
O,O-diethyl hydrogen phosphorodithioate	247-571-4	26266-68-2	26266682	2459	Reach_2577	2597	3.79	1.34	3				-6.5	-6.3	-7.3	0.0%	0.0%	0.0%
5-nitro-o-toluidine	255-419-3	41506-62-1	41506621	2879	Reach_2744	2598	5.70		1				-5.9	-6.3	-7.1	0.0%	0.0%	0.0%
2,5-diaminobenzenesulphonic acid	246-141-3	24304-50-5	24304505	2385	Reach_2544	2599	4.35	1.12	3				-5.3	-6.3	-7.9	0.0%	0.0%	0.0%
2,2'-(cyclohexylimino)bisethanol	224-809-5	4500-29-2	4500292	2936	Reach_2043	2600	5.04	0.57	3	4.04	0.57		-5.6	-6.3	-7.9	0.0%	0.0%	0.0%
ethyl 2-[3-cyano-4-(2-methylpropoxy)phenyl]-4-methyl-1,3-thiaz	206-055-9	298-06-6	298066	591	Reach_1226	2601	5.16	1.52	3	4.16	1.52		-5.9	-6.3	-7.9	0.0%	0.0%	0.0%
610-147-8	604-200-4	14078-41-2	14078412	1930	Reach_4144	2602	5.42	0.25	3	4.42	0.25		-5.4	-6.3	-7.9	0.0%	0.0%	0.0%
619-914-1	694-989-1	41131-49-1	41131491	5876	Reach_4685	2603							-5.4	-6.3	-7.9	0.0%	0.0%	0.0%
cis-2-tert-butylcyclohexyl acetate	243-718-1	20298-69-5	20298695	2258	Reach_2492	2604	3.87	0.32	3	2.87	0.32		-6.5	-6.3	-8.8	0.0%	0.0%	0.0%
ethyl phenyl(2,4,6-trimethylbenzoyl)phosphinate	805-107-3	40758-65-4	40758654	2865	Reach_5059	2605	3.93	0.56	3	2.93	0.56		-6.3	-6.3	-7.9	0.0%	0.0%	0.0%
propane-1,2,3-triyl trisheptanoate	210-647-2	620-67-7	620677	3361	Reach_1441	2606	2.21	0.04	3	3.80			-5.9	-6.3	-7.1	0.0%	0.0%	0.0%
1-(2,3-Dichlorophenyl)piperazine hydrochloride	202-940-9	101-41-7	101417	1321	Reach_577	2607	5.11	0.49	3	4.11	0.49		-6.0	-6.3	-7.6	0.0%	0.0%	0.0%
1,4-dioxacyclohexadecane-5,16-dione	259-423-6	54982-83-1	54982831	3157	Reach_2804	2608	3.35		2				-6.5	-6.3	-7.5	0.0%	0.0%	0.0%
5-(2-chloroethyl)-4-methyl-1,3-thiazole hydrochloride (1:1)	247-501-2	26175-68-8	26175688	2456	Reach_2576	2609	4.04	0.62	3				-6.0	-6.3	-7.6	0.0%	0.0%	0.0%
trichlorotrifluoroethane	614-284-4	68127-98-0	68127980	3506	Reach_4397	2610	4.44	0.76	3				-6.7	-6.3	-8.5	0.0%	0.0%	0.0%
Ethyl 2-methylbut-3-enoate	211-550-8	661-95-0	661950	3466	Reach_1492	2611	3.97	0.11	3				-6.5	-6.3	-7.8	0.0%	0.0%	0.0%
2-ethoxyphenol	202-358-5	94-71-3	94713	4111	Reach_418	2612	4.30		1				-6.5	-6.3	-7.8	0.0%	0.0%	0.0%
N-isopropylhydroxylamine	214-244-2	1117-31-3	1117313	1555	Reach_1650	2613	5.26	0.29	3	4.26	0.29		-6.4	-6.3	-7.8	0.0%	0.0%	0.0%
[3-(triethoxysilyl)propyl]urea	245-876-7	23779-32-0	23779320	2358	Reach_2534	2614	5.17	0.58	3	4.17	0.58		-5.6	-6.3	-8.0	0.0%	0.0%	0.0%
N-(1,4-dimethylpentyl)-N'-phenylbenzene-1,4-diamine	221-374-3	3081-01-4	3081014	1257	Reach_1912	2615	3.26	1.22	3	2.26	1.22		-5.9	-6.3	-7.9	0.0%	0.0%	0.0%
4-nitro-m-xylene	231-274-1	7474-78-4	7474784	3643	Reach_2254	2616	4.94		1				-6.5	-6.3	-7.6	0.0%	0.0%	0.0%
bromotrifluoromethane	200-887-6	75-63-8	75638	3678	Reach_154	2617	4.69	0.27	3				-6.6	-6.3	-8.6	0.0%	0.0%	0.0%
diisobutyl hexahydrophthalate	275-069-5	70969-58-3	70969583	815	Reach_2924	2618	3.12	0.38	3	2.80	0.38		-6.5	-6.3	-7.5	0.0%	0.0%	0.0%
600-198-4	222-646-4	3564-28-1	3564281	5856	Reach_1972	2619							-5.9	-6.3	-7.9	0.0%	0.0%	0.0%
p-aminobenzamide	608-301-4	2896-99-3	2896993	2552	Reach_4270	2620	3.16	0.63	3				-5.5	-6.3	-7.9	0.0%	0.0%	0.0%
607-929-6	700-516-2	93413-62-8	93413628	4069	Reach_4917	2621	4.13	0.34	3	3.13	0.34		-6.2	-6.3	-7.9	0.0%	0.0%	0.0%
3'-(trifluoromethyl)acetophenone	258-556-7	53445-37-7	53445377	3103	Reach_2793	2622	5.12	0.43	3	4.12	0.43		-6.5	-6.3	-7.6	0.0%	0.0%	0.0%
613-198-4	613-198-4	63302-43-2	63302432	3397	Reach_4384	2623	3.37	0.37	3				-6.4	-6.3	-7.9	0.0%	0.0%	0.0%
2',3-bis[[3-[3,5-di-tert-butyl-4-hydroxyphenyl]propionyl]]propion	251-156-3	32687-78-8	32687788	2659	Reach_2664	2624	4.24		2				-5.8	-6.3	-7.0	0.0%	0.0%	0.0%
3,5-diamino-2,4,6-triiodobenzoic acid	619-914-1	1116495-86-3	1116495863	1552	Reach_4554	2625	4.19	0.87	3				-5.6	-6.3	-7.9	0.0%	0.0%	0.0%
6-methyloct-5-en-2-one	213-382-0	941-69-5	941695	4098	Reach_1614	2626	2.87	0.27	3	1.90	0.25		-6.5	-6.3	-7.6	0.0%	0.0%	0.0%
616-390-6	616-390-6	76811-98-8	76811988	3724	Reach_4437	2627	2.16	1.13	3				-5.7	-6.3	-7.9	0.0%	0.0%	0.0%
801-014-7	801-014-7	179107-88-1	179107881	2157	Reach_5050	2628	2.98	0.72	3				-6.5	-6.3	-7.5	0.0%	0.0%	0.0%
1-[bis[3-(dimethylamino)propyl]amino]propan-2-ol	266-587-2	67151-63-7	67151637	3487	Reach_2885	2629	4.70	0.41	3	3.70	0.41		-5.4	-6.3	-8.1	0.0%	0.0%	0.0%
617-349-5	617-589-0	84592-32-5	84592325	6053	Reach_4468	2630	4.13		2				-5.6	-6.3	-7.9	0.0%	0.0%	0.0%
heptan-1-ol	203-897-9	111-70-6	111706	308	Reach_866	2631	4.81	0.36	29	3.81	0.36	29	-6.5	-6.3	-7.6	0.0%	0.0%	0.0%
Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]l	271-878-2	68610-86-6	68610866	3522	Reach_2909	2632	5.26	1.21	3	4.26	1.21		-5.8	-6.3	-7.1	0.0%	0.0%	0.0%
6-[(1S)-1,3-dihydroxy-1-(1-trityl-1H-imidazol-4-yl)propyl]-N-meth	700-333-8	1021394-33-1	1021394331	1337	Reach_4865	2633	2.08		1				-5.9	-6.3	-7.6	0.0%	0.0%	0.0%
614-070-0	608-307-7	2901-13-5	2901135	2555	Reach_4271	2634	4.42		2				-5.7	-6.3	-7.9	0.0%	0.0%	0.0%
(Z)-[cyano(2,3-dichlorophenyl)methylene]carbazamidine	700-837-8	1093205-95-8	1093205958	1499	Reach_5005	2635	4.31	1.26	3				-5.7	-6.3	-7.6	0.0%	0.0%	0.0%
vinyl 2-ethylhexanoate	202-297-4	94-04-2	94042	4096	Reach_410	2636	3.10	0.44	3	2.62	0.32		-6.5	-6.3	-7.9	0.0%	0.0%	0.0%
dodecamethylpentasiloxane	275-662-9	71604-74-5	71604745	3586	Reach_2928	2637	4.22	0.32	3	3.52	0.35		-6.5	-6.3	-7.2	0.0%	0.0%	0.0%
4-hydroxymethyl-1,3-dioxolan-2-one	213-235-0	931-40-8	931408	4060	Reach_1608	2638	6.12		2				-5.4	-6.3	-8.0	0.0%	0.0%	0.0%
o-(trifluoromethyl)benzaldehyde	209-840-4	594-42-3	594423	3276	Reach_1398	2639	4.06	0.15	3				-6.5	-6.3	-7.6	0.0%	0.0%	0.0%
tert-butyl α,α-dimethylbenzyl peroxide	222-389-8	3457-61-2	3457612	2709	Reach_1965	2640	3.63		1				-6.5	-6.3	-7.4	0.0%	0.0%	0.0%
1,4-bis[(2-ethyl-6-methylphenyl)amino]anthraquinone	255-460-7	41611-76-1	41611761	2881	Reach_2745	2641	4.93		1				-6.4	-6.3	-6.7	0.0%	0.0%	0.0%
(5-ethyl-1,3-dioxan-5-yl)methyl acrylate	266-380-7	66492-51-1	66492511	3475	Reach_2882	2642	3.90	0.47	3	2.90	0.47		-6.5	-6.3	-7.9	0.0%	0.0%	0.0%
5,6-Di-tert-butyl-21-({tert-butyl[1-(diethoxyphosphoryl)-2,2-dim	629-671-3	1522-41-4	1522414	2022	Reach_4594	2643	4.33	1.36	3				-6.0	-6.3	-7.7	0.0%	0.0%	0.0%

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Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
bis(triphenylphosphine)nickel(II) chloride	700-562-3	909782-32-7	909782327	4009	Reach_4935	2644	3.91	0.39	3				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
Benzoic acid, 2-hydroxy-5-sulfo-, compd. with [4S-(4α,4aα,5α,5a	205-811-5	152-97-6	152976	2026	Reach_1209	2645	4.56	0.37	3				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
617-385-1	238-154-8	14264-16-5	14264165	6395	Reach_2362	2646							-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
2,4,4-trimethylpentan-2-aminium (3R,5S,6E)-7-{4-(4-fluorophen	700-704-4	923036-25-3	923036253	4031	Reach_4974	2647	2.61	0.30	3				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
Adenosine 5'-(trihydrogen diphosphate), 2'-(dihydrogen phosph	246-129-8	24292-60-2	24292602	5790	Reach_2542	2648							-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
[3-(dimethylamino)propyl](triphenyl)phosphonium bromide hyd	923-250-0	156755-23-6	156755236	2050	Reach_5098	2649	3.15	0.51	3				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
dichloro(methyl)(phenyl)silane	205-746-2	149-74-6	149746	2006	Reach_1202	2650	5.01	0.70	3	4.01	0.70		-6.5	-6.3	-7.6	0.0%	0.0%	0.0%
calcium N2,N6-bis(3-carboxypropanoyl)lysine (1:1)	700-699-9	877397-65-4	877397654	3940	Reach_4972	2651	3.69	0.50	3				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
N,N-Dibenzyl-N-[2-(3,4-dihydroxyphenyl)-2-oxoethyl]ammonium	613-308-0	63659-15-4	63659154	3415	Reach_4385	2652	3.33	0.06	3				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
2-({6-[(3R)-3-Aminopiperidin-1-yl]-3-methyl-2,4-dioxo-3,4-dihydr	700-046-8	16004-15-2	16004152	2071	Reach_4738	2653							-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
4-methoxy-3,5-dimethylpyridine-2-methanol	289-258-5	86604-78-6	86604786	3908	Reach_2990	2654	4.48	0.86	3				-5.6	-6.3	-8.0	0.0%	0.0%	0.0%
618-311-0	692-179-2	161798-01-2	161798012	2081	Reach_4674	2655	3.53	0.30	3				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
1-bromohexadecane	204-008-7	112-82-3	112823	1606	Reach_925	2656							-6.2	-6.3	-7.8	0.0%	0.0%	0.0%
4-chlorobutyryl chloride	214-093-2	1079-66-9	1079669	1474	Reach_1644	2657	4.76		2				-6.6	-6.3	-7.9	0.0%	0.0%	0.0%
pyruvaldehyde	201-164-8	78-98-8	78988	3763	Reach_221	2658	5.82	0.20	3	4.98	0.33		-6.5	-6.3	-7.8	0.0%	0.0%	0.0%
4-(cyclohexylcarbonoimidoyl)-5-(hydroxymethyl)-2-methylpyridi	700-068-8	103953-71-5	103953715	1381	Reach_4749	2659	3.55	0.84	3				-5.7	-6.3	-7.9	0.0%	0.0%	0.0%
3-[(dimethylamino)methyl]-9-methyl-1,2,3,9-tetrahydro-4H-carb	216-613-3	1624-62-0	1624620	2084	Reach_1700	2660	1.60		1				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
(3R,4R)-1-benzyl-N,4-dimethylpiperidin-3-amine dihydrochloride	700-215-6	165670-57-5	165670575	2101	Reach_4807	2661	3.38	0.17	3				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
2-(1-hydroxycyclohexyl)-2-(4-methoxyphenyl)ethyl ammonium c	618-311-0	898543-06-1	898543061	6078	Reach_4493	2662							-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
N,N,N-tripropylprop-2-en-1-aminium dicyanoazanide	700-603-5	908145-87-9	908145879	4007	Reach_4949	2663	3.75	0.81	3				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
p-(trifluoromethoxy)phenyl isocyanate	252-328-0	35037-73-1	35037731	2720	Reach_2685	2664	4.29		1				-6.6	-6.3	-8.3	0.0%	0.0%	0.0%
(2,2,8-trimethyl-4H-[1,3]dioxino[4,5-c]pyridin-5-yl)methanol hyd	240-722-5	16673-34-0	16673340	2109	Reach_2426	2665	3.76	0.80	3				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
1,3-bis(allylamino)propan-2-ol dihydrochloride	605-530-1	16874-33-2	16874332	2114	Reach_4177	2666	5.70	0.59	3				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
2-aminododecan-1-ol hydrochloride (1:1)	246-403-7	24683-26-9	24683269	2401	Reach_2553	2667							-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
606-318-1	628-731-6	17159-79-4	17159794	2123	Reach_4588	2668	4.60	1.00	3				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
2-(1-hydroxy-1-phenylethyl)pyridinium chloride	242-005-2	18109-80-3	18109803	2165	Reach_2451	2669	3.63	0.65	3				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
1-ethyl-3-methyl-1H-imidazolium methanesulfonate (1:1)	226-137-8	5292-53-5	5292535	3081	Reach_2095	2670	3.47	0.26	3				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
(3-chloro-4-methoxyphenyl)methanaminium chloride	700-268-5	18143-33-4	18143334	2167	Reach_4831	2671							-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
phenylephrine hydrochloride	202-993-8	101-97-3	101973	1332	Reach_586	2672	4.01	0.80	3				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
2-(2-methoxy-phenoxy)ethylammonium chloride	245-371-1	22990-77-8	22990778	2342	Reach_2526	2673	4.59	0.94	3				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
Sodium 4-fluorobenzenesulfinate	807-096-0	917805-85-7	917805857	6082	Reach_5082	2674							-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
615-083-4	219-397-9	2431-50-7	2431507	2386	Reach_1807	2675	4.07	1.08	3	3.07	1.08		-5.7	-6.3	-7.9	0.0%	0.0%	0.0%
2-butyloctan-1-ol	223-470-0	3913-02-8	3913028	1263	Reach_2001	2676	3.79	1.60	3	1.76	1.14		-6.5	-6.3	-7.5	0.0%	0.0%	0.0%
mesitylene	201-099-5	78-26-2	78262	3749	Reach_196	2677	5.44	0.50	3				-6.6	-6.3	-8.1	0.0%	0.0%	0.0%
1,1'-[[3-(dimethylamino)propyl]imino]bispropan-2-ol	619-573-9	855425-38-6	855425386	3892	Reach_4530	2678	2.16		1				-5.5	-6.3	-8.1	0.0%	0.0%	0.0%
613-147-6	200-638-1	66-84-2	66842	5984	Reach_79	2679							-6.5	-6.3	-7.6	0.0%	0.0%	0.0%
1,5-dihydro-3-isopropyl-8-methyl-[1,3]dioxepino[5,6-c]pyridin-9-	249-922-7	29878-91-9	29878919	2576	Reach_2634	2680	2.41	0.68	3				-5.8	-6.3	-7.9	0.0%	0.0%	0.0%
bumetrizole	223-445-4	3896-11-5	3896115	1262	Reach_1998	2681	5.00		1				-5.7	-6.3	-7.9	0.0%	0.0%	0.0%
phenylephrine	700-018-5	50892-62-1	50892621	3020	Reach_4726	2682	3.24	0.69	3				-5.6	-6.3	-8.0	0.0%	0.0%	0.0%
tert-butyl isocyanate	201-874-8	89-00-9	89009	3966	Reach_336	2683							-6.5	-6.3	-7.5	0.0%	0.0%	0.0%
2-[(2-methyl-1-oxoallyl)oxy]ethyl acetoacetate	211-560-2	665-66-7	665667	5981	Reach_1493	2684	4.53	0.23	3	3.53	0.23		-6.5	-6.3	-8.0	0.0%	0.0%	0.0%
methyl 4-methyl-3-{[4-(pyridin-3-yl)pyrimidin-2-yl]amino}benzoa	939-899-8	1441670-89-8	1441670898	1973	Reach_5161	2685	2.69	0.72	3				-5.8	-6.3	-7.9	0.0%	0.0%	0.0%
nonan-1-ol	264-347-1	63589-25-3	63589253	3412	Reach_2861	2686	5.40		1				-6.5	-6.3	-7.7	0.0%	0.0%	0.0%
N-[4-(acetylamino)phenyl]-4-[[5-(aminocarbonyl)-2-chlorophen	243-737-5	20325-40-0	20325400	5767	Reach_2493	2687							-6.1	-6.3	-7.9	0.0%	0.0%	0.0%
3,7-dimethyloct-6-en-1-yn-3-ol	249-482-6	29171-20-8	29171208	2560	Reach_2628	2688	4.62	0.10	3	3.74	0.19		-6.5	-6.3	-7.6	0.0%	0.0%	0.0%
3-methoxybutyl acetate	224-644-9	4435-53-4	4435534	2923	Reach_2036	2689	4.59		2				-6.5	-6.3	-7.7	0.0%	0.0%	0.0%
pentadecan-15-olide	203-354-6	106-02-5	106025	1425	Reach_654	2690	3.42	0.48	3	2.26	0.43		-6.4	-6.3	-7.5	0.0%	0.0%	0.0%
ethyl methacrylate	202-597-5	97-63-2	97632	4167	Reach_483	2691	4.57	1.14	3	3.87	1.36		-6.6	-6.3	-7.8	0.0%	0.0%	0.0%
thiophene	689-247-9	95149-35-2	95149352	4121	Reach_4649	2692	1.84	0.33	3				-6.6	-6.3	-8.2	0.0%	0.0%	0.0%
L-serine	200-274-3	56-45-1	56451	3199	Reach_29	2693	7.69		1				-5.3	-6.3	-7.9	0.0%	0.0%	0.0%
2-methylvaleric acid	219-823-3	2544-13-0	2544130	5797	Reach_1834	2694							-6.2	-6.3	-7.9	0.0%	0.0%	0.0%
4-phenylbutenone	204-555-1	122-57-6	122576	1752	Reach_1031	2695	4.74	0.59	3	3.74	0.59		-6.5	-6.3	-7.8	0.0%	0.0%	0.0%
2-nitro-p-xylene	616-206-4	7529-16-0	7529160	3662	Reach_4426	2696	4.28	1.32	3				-6.5	-6.3	-7.7	0.0%	0.0%	0.0%
615-161-8	201-744-0	87-41-2	87412	3932	Reach_309	2697	5.45		1				-6.6	-6.3	-8.1	0.0%	0.0%	0.0%
decahydronaphthalene	203-874-3	111-48-8	111488	1549	Reach_859	2698	6.12	0.57	3				-6.6	-6.3	-8.5	0.0%	0.0%	0.0%
p-[(2-chloroethyl)ethylamino]benzaldehyde	220-150-2	2643-07-4	2643074	1253	Reach_1850	2699	3.44	0.61	3	2.51	0.44		-5.9	-6.3	-7.9	0.0%	0.0%	0.0%
tert-butyl peroxypivalate	213-147-2	927-07-1	927071	4046	Reach_1599	2700	3.67	0.73	3	2.76	0.85		-6.6	-6.3	-8.1	0.0%	0.0%	0.0%
2,4-xylenol	203-635-3	108-98-5	108985	1491	Reach_766	2701	1.46	1.11	3	0.46	1.11		-6.6	-6.3	-7.5	0.0%	0.0%	0.0%
3-methylbutanone	209-264-3	563-80-4	563804	712	Reach_1375	2702	5.16	0.34	3	4.16	0.34		-6.6	-6.3	-7.7	0.0%	0.0%	0.0%
1-(tetrahydrofuran-3-yl)methanamine	255-235-3	41131-65-1	41131651	2870	Reach_2736	2703	4.32	1.12	3				-6.5	-6.3	-7.7	0.0%	0.0%	0.0%
2-Propylheptan-1-amine	620-520-7	194608-78-1	194608781	2234	Reach_4575	2704	3.80		1				-6.6	-6.3	-8.0	0.0%	0.0%	0.0%
bisdecanoyl peroxide	212-092-1	762-12-9	762129	3706	Reach_1535	2705	0.97	0.67	3				-6.2	-6.3	-7.6	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
cyclopropanecarbonyl chloride	689-242-1	95149-34-1	95149341	4120	Reach_4648	2706	2.22	0.21	3				-6.6	-6.3	-7.7	0.0%	0.0%	0.0%
triethylammonium bromide	211-263-8	636-70-4	636704	5963	Reach_1475	2707	5.11		1				-6.1	-6.3	-7.7	0.0%	0.0%	0.0%
2,6-di-tert-butyl-α-dimethylamino-p-cresol	201-816-1	88-27-7	88277	3954	Reach_322	2708	2.93	0.33	3	1.93	0.33		-6.5	-6.3	-7.8	0.0%	0.0%	0.0%
2-Chloro-3-(2,2,2-trifluoroethoxy)pyridine.	608-497-1	3056-13-1	3056131	2603	Reach_4276	2709	2.88	0.40	3				-6.6	-6.4	-7.8	0.0%	0.0%	0.0%
tetraethylammonium heptadecafluorooctanesulphonate	609-106-7	35249-89-9	35249899	5855	Reach_4289	2710	4.82		2				-6.1	-6.4	-7.7	0.0%	0.0%	0.0%
penta-1,3-diene	207-995-2	504-60-9	504609	3006	Reach_1305	2711	4.24	0.25	3				-6.6	-6.4	-8.8	0.0%	0.0%	0.0%
1-{[(6R,7R)-7-amino-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]o	700-425-8	521284-22-0	521284220	3053	Reach_4898	2712	4.02		2				-6.1	-6.4	-7.7	0.0%	0.0%	0.0%
607-985-1	613-004-8	62285-89-6	62285896	5955	Reach_4378	2713	3.56		1				-5.7	-6.4	-7.9	0.0%	0.0%	0.0%
trichloromethanesulphenyl chloride	700-054-1	70905-68-9	70905689	3574	Reach_4742	2714	3.67	0.77	3				-6.6	-6.4	-8.3	0.0%	0.0%	0.0%
4-acetyl-1-methylpyridinium 4-methylbenzenesulfonate	298-613-3	93820-33-8	93820338	4086	Reach_2998	2715	1.90	0.11	3				-6.1	-6.4	-7.7	0.0%	0.0%	0.0%
O-isopropyl ethylthiocarbamate	205-517-7	141-98-0	141980	460	Reach_1171	2716	4.63	0.22	4	3.63	0.22		-6.6	-6.4	-7.4	0.0%	0.0%	0.0%
lithium 3-[(3,4-dicyanophenyl)sulfanyl]propane-1-sulfonate.	606-216-7	190651-18-4	190651184	5753	Reach_4198	2717							-6.1	-6.4	-7.7	0.0%	0.0%	0.0%
2-[(3-aminopyrazolo[1,5-a]pyridin-2-yl)oxy]ethanol hydrochlorid	254-235-0	38982-12-6	38982126	2830	Reach_2721	2718	2.60	0.32	3				-6.1	-6.4	-7.7	0.0%	0.0%	0.0%
Trisodium [carboxy(oxido)methyl]phosphonate	695-745-7	1079221-49-0	1079221490	5604	Reach_4695	2719	3.64		2				-6.1	-6.4	-7.7	0.0%	0.0%	0.0%
2,6-dimethylcyclohexylamine	700-167-6	94695-50-8	94695508	4108	Reach_4787	2720	3.65	0.72	3				-6.6	-6.4	-8.2	0.0%	0.0%	0.0%
dimethyl [3-chloro-5-(trifluoromethyl)pyridin-2-yl]({[2-(trifluoron	247-628-3	26351-32-6	26351326	2466	Reach_2580	2721	1.39	0.20	3				-5.9	-6.4	-7.7	0.0%	0.0%	0.0%
chloro(3-chloropropyl)dimethylsilane	700-310-2	71839-12-8	71839128	3592	Reach_4854	2722	3.47	0.68	3				-6.6	-6.4	-8.3	0.0%	0.0%	0.0%
2-phenylisobutyric acid	201-497-9	83-73-8	83738	3850	Reach_284	2723	4.10	0.15	3	3.10	0.15		-5.7	-6.4	-8.0	0.0%	0.0%	0.0%
2,2-dimethylbutyryl chloride	227-478-5	5856-77-9	5856779	3250	Reach_2138	2724	4.34	0.45	3				-6.6	-6.4	-8.0	0.0%	0.0%	0.0%
etilefrine	206-490-4	349-76-8	349768	2719	Reach_1241	2725	3.53	1.07	3				-5.6	-6.4	-8.0	0.0%	0.0%	0.0%
Ammonium glycolate	619-072-5	94744-50-0	94744500	4113	Reach_4510	2726	3.62	0.24	3				-6.1	-6.4	-7.7	0.0%	0.0%	0.0%
DL-lysine	212-201-2	768-94-5	768945	878	Reach_1543	2727	4.49	0.20	4	3.49	0.20		-5.3	-6.4	-8.1	0.0%	0.0%	0.0%
3,4-dimethoxy-N-methylphenethylamine	262-828-0	61516-73-2	61516732	3337	Reach_2850	2728	4.34	1.42	3				-6.6	-6.4	-7.9	0.0%	0.0%	0.0%
citraconic anhydride	210-459-0	616-02-4	616024	3341	Reach_1429	2729	4.73	1.14	3				-6.6	-6.4	-7.9	0.0%	0.0%	0.0%
veratrole	202-045-3	91-16-7	91167	4013	Reach_370	2730	4.51		1				-6.6	-6.4	-7.6	0.0%	0.0%	0.0%
3-(trifluoromethyl)benzoyl fluoride	226-518-9	5417-35-6	5417356	3130	Reach_2107	2731	5.88		1				-6.6	-6.4	-7.9	0.0%	0.0%	0.0%
butane-1,4-disulfonic acid	269-507-4	68259-05-2	68259052	3513	Reach_2903	2732	-0.48	3.08	3	4.00			-5.3	-6.4	-8.1	0.0%	0.0%	0.0%
cyclohexylethylcarbamoyl chloride	263-753-6	62899-75-6	62899756	3383	Reach_2855	2733	3.69	0.86	3				-6.6	-6.4	-7.9	0.0%	0.0%	0.0%
decamethyltetrasiloxane	204-606-8	123-17-1	123171	1764	Reach_1041	2734	3.14	0.27	3	2.14	0.27		-6.5	-6.4	-7.8	0.0%	0.0%	0.0%
609-335-2	600-024-7	1000777-61-6	1000777616	5589	Reach_4054	2735	4.68	0.35	3	3.68	0.35		-6.6	-6.4	-7.4	0.0%	0.0%	0.0%
2-methylbut-3-en-2-ol	204-068-4	115-18-4	115184	1632	Reach_938	2736	6.50		1				-6.6	-6.4	-7.6	0.0%	0.0%	0.0%
Tetrahydropyran-4-carboxaldehyde	700-032-1	50675-18-8	50675188	3015	Reach_4732	2737	5.81		1				-6.6	-6.4	-7.9	0.0%	0.0%	0.0%
bis(2-ethylhexyl)amine	203-372-4	106-20-7	106207	1430	Reach_657	2738	3.29	0.51	3	2.01	0.73		-6.6	-6.4	-8.6	0.0%	0.0%	0.0%
[4-[4,4'-bis(dimethylamino)benzhydrylidene]cyclohexa-2,5-dien-	208-953-6	548-62-9	548629	1220	Reach_1356	2739	2.23	0.28	3	1.23	0.28		-6.1	-6.4	-7.7	0.0%	0.0%	0.0%
2-(4-bromophenyl)-2-methylpropanoic acid	212-556-3	826-55-1	826551	3835	Reach_1557	2740	4.16		2				-5.9	-6.4	-8.0	0.0%	0.0%	0.0%
o-fluoro-α,α,α-trichlorotoluene	700-273-2	39627-98-0	39627980	2844	Reach_4833	2741	3.43	0.79	3				-6.6	-6.4	-8.1	0.0%	0.0%	0.0%
bromochloromethane	200-826-3	74-97-5	74975	844	Reach_120	2742	4.83	0.70	4	3.83	0.70		-6.6	-6.4	-8.1	0.0%	0.0%	0.0%
dimethyl(octyl)amine	230-939-3	7378-99-6	7378996	833	Reach_2242	2743	3.92		2				-6.6	-6.4	-8.1	0.0%	0.0%	0.0%
3-diethylaminopropiononitrile	617-349-5	82543-17-7	82543177	3830	Reach_4456	2744	5.75	1.88	3				-6.6	-6.4	-7.9	0.0%	0.0%	0.0%
α,α,α-trifluoro-o-toluidine	201-806-7	88-17-5	88175	3949	Reach_317	2745	4.24		2				-6.4	-6.4	-7.9	0.0%	0.0%	0.0%
octane	201-873-2	88-99-3	88993	990	Reach_335	2746	5.58	0.60	4	4.68	0.44		-6.6	-6.4	-8.7	0.0%	0.0%	0.0%
1-bromo-4-fluorobenzene	612-012-9	60728-43-0	60728430	3315	Reach_4370	2747	2.80	1.05	3				-6.6	-6.4	-8.2	0.0%	0.0%	0.0%
2-chlorobutane	201-151-7	78-86-4	78864	3760	Reach_212	2748	5.12	0.41	3	4.12	0.41		-6.6	-6.4	-8.6	0.0%	0.0%	0.0%
1,2,3-Trichloro-5-(trichloromethyl)benzene	291-751-5	90474-13-8	90474138	4000	Reach_2994	2749	4.67	0.29	3	3.67	0.29		-6.6	-6.4	-8.1	0.0%	0.0%	0.0%
thiodi(acetic acid)	204-663-9	123-93-3	123933	1777	Reach_1062	2750	5.05	0.91	3				-5.4	-6.4	-8.0	0.0%	0.0%	0.0%
2,2-dimethylpropane-1,3-diyl 2-ethylhexanoate	249-060-1	28510-23-8	28510238	2534	Reach_2619	2751	2.20		1				-6.5	-6.4	-8.1	0.0%	0.0%	0.0%
p-cymene	202-796-7	99-87-6	99876	1092	Reach_540	2752	4.33	0.70	20	3.33	0.70		-6.6	-6.4	-8.3	0.0%	0.0%	0.0%
615-275-8	617-834-1	863329-69-5	863329695	3904	Reach_4474	2753	3.43	0.14	3				-6.4	-6.4	-7.9	0.0%	0.0%	0.0%
propiophenone	202-257-6	93-55-0	93550	4072	Reach_402	2754	4.24	0.69	3				-6.6	-6.4	-7.4	0.0%	0.0%	0.0%
2-butylaminoethanol	201-089-0	78-16-0	78160	3748	Reach_195	2755	2.77		1	6.41			-6.3	-6.4	-8.0	0.0%	0.0%	0.0%
1,2,4-triazolo[4,3-a]pyridin-3(2H)-one	241-866-1	17927-72-9	17927729	5744	Reach_2447	2756	5.62	0.35	3	4.62	0.35		-5.7	-6.4	-8.0	0.0%	0.0%	0.0%
N,N-bis[3-(dimethylamino)propyl]-N',N'-dimethylpropane-1,3-di	251-459-0	33329-35-0	33329350	2680	Reach_2668	2757	4.76	0.53	3	3.76	0.53		-5.8	-6.4	-8.2	0.0%	0.0%	0.0%
dimethyl 5-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]	244-815-1	22174-70-5	22174705	2322	Reach_2518	2758	4.17		1				-5.7	-6.4	-8.0	0.0%	0.0%	0.0%
619-015-4	619-015-4	943516-53-8	943516538	4101	Reach_4507	2759	3.06	0.83	3				-5.8	-6.4	-7.9	0.0%	0.0%	0.0%
(2S)-2-Benzyl-N,N-dimethylaziridine-1-sulfonamide	700-257-5	31251-41-9	31251419	2622	Reach_4826	2760	3.66	0.12	3				-5.7	-6.4	-7.9	0.0%	0.0%	0.0%
oxydiethylene dinitrate	212-603-8	831-52-7	831527	6046	Reach_1560	2761	5.30	0.56	3	4.30	0.56		-6.5	-6.4	-8.1	0.0%	0.0%	0.0%
2-ethylhexyl (3-isocyanatomethylphenyl)-carbamate	208-066-4	507-20-0	507200	3017	Reach_1316	2762	5.43		2				-6.4	-6.4	-7.7	0.0%	0.0%	0.0%
ethylene diacetoacetate	200-306-6	57-00-1	57001	3220	Reach_35	2763	4.74	0.96	3				-6.2	-6.4	-8.2	0.0%	0.0%	0.0%
cyclohexylidenebis[tert-butyl] peroxide	221-111-2	3006-86-8	3006868	2584	Reach_1896	2764	3.43	1.04	3				-6.5	-6.4	-7.4	0.0%	0.0%	0.0%
m-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	205-492-2	141-63-9	141639	1940	Reach_1166	2765	0.00	0.66	3	-1.00	0.66		-5.6	-6.4	-8.1	0.0%	0.0%	0.0%
7-aminonaphthalene-1,3,5-trisulphonic acid	248-394-5	27310-25-4	27310254	2500	Reach_2600	2766	5.32	1.39	3				-5.4	-6.4	-8.0	0.0%	0.0%	0.0%
butyryl chloride	217-547-8	1885-14-9	1885149	2212	Reach_1731	2767	4.03		1				-6.6	-6.4	-8.1	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
2-(m-benzoylphenyl)propionitrile	225-302-1	4763-40-0	4763400	2968	Reach_2062	2768	2.40	0.67	3				-6.5	-6.4	-7.9	0.0%	0.0%	0.0%
p-tert-butylcinnamaldehyde	282-823-7	84434-23-1	84434231	3865	Reach_2975	2769	3.26		1				-6.6	-6.4	-7.5	0.0%	0.0%	0.0%
methyl 2-chloropropionate	241-624-5	17639-93-9	17639939	2147	Reach_2440	2770	4.49	1.90	3				-6.6	-6.4	-7.8	0.0%	0.0%	0.0%
2,6,6-trimethylcyclohex-2-ene-1,4-dione	240-734-0	16690-93-0	16690930	5736	Reach_2427	2771	5.62		2				-6.6	-6.4	-7.9	0.0%	0.0%	0.0%
α,α,α-trifluoro-3-tolyl isocyanate	206-341-3	329-01-1	329011	2668	Reach_1237	2772	3.99	0.43	3	3.58	0.38		-6.6	-6.4	-8.0	0.0%	0.0%	0.0%
dibutyl ether	205-575-3	142-96-1	142961	467	Reach_1187	2773	4.84	0.45	7	3.84	0.45		-6.6	-6.4	-8.2	0.0%	0.0%	0.0%
methyl cholate	215-903-7	1448-36-8	1448368	1982	Reach_1681	2774	3.45		2				-5.7	-6.4	-7.9	0.0%	0.0%	0.0%
[[(phosphonomethyl)imino]bis[ethylenenitrilobis(methylene)]]te	700-525-1	54090-39-0	54090390	3123	Reach_4920	2775	2.49	0.42	3				-6.1	-6.4	-7.8	0.0%	0.0%	0.0%
tert-butyl 3-[6-({[1-(2,2-difluoro-1,3-benzodioxol-5-yl)cyclopropy	204-501-7	121-86-8	121868	376	Reach_1020	2776	3.91	0.70	16	2.91	0.70		-5.6	-6.4	-7.9	0.0%	0.0%	0.0%
phthalylsulfathiazole	696-555-7	32454-35-6	32454356	2652	Reach_4719	2777	3.41		2				-5.8	-6.4	-8.0	0.0%	0.0%	0.0%
620-459-6	620-459-6	130841-23-5	130841235	1844	Reach_4569	2778	2.29	0.45	3	1.13	0.75		-6.6	-6.4	-7.9	0.0%	0.0%	0.0%
N-[2-[(2-hydroxyethyl)amino]ethyl]dodecanamide	235-930-8	13051-49-5	13051495	1838	Reach_2321	2779	4.94		1				-5.8	-6.4	-7.9	0.0%	0.0%	0.0%
4-(4-iodo-1H-pyrazol-1-yl)piperidine	609-304-3	368890-20-4	368890204	2784	Reach_4296	2780	2.58	0.29	3				-5.8	-6.4	-8.0	0.0%	0.0%	0.0%
N-phenylbenzenesulphonamide	608-993-8	34455-22-6	34455226	2707	Reach_4286	2781	3.44	0.34	3				-6.0	-6.4	-7.9	0.0%	0.0%	0.0%
1-[(2E)-3,7-dimethylocta-2,6-dien-1-yl]pyrrolidine-2,5-dione	800-131-0	104372-31-8	104372318	1392	Reach_5037	2782	4.49	1.27	3				-5.8	-6.4	-7.9	0.0%	0.0%	0.0%
(E)-3,7-dimethylocta-2,6-dienal	219-194-5	2385-77-5	2385775	2361	Reach_1791	2783	4.09	0.23	3	3.12	0.37		-6.6	-6.4	-7.8	0.0%	0.0%	0.0%
(Z)-3,7-dimethylocta-2,6-dienal	205-476-5	141-27-5	141275	1935	Reach_1160	2784	4.23	0.68	3	3.05	0.10		-6.6	-6.4	-7.8	0.0%	0.0%	0.0%
tetradecyl acrylate	244-491-1	21643-42-5	21643425	2302	Reach_2507	2785	4.60	0.92	3	3.37	1.08		-6.5	-6.4	-7.9	0.0%	0.0%	0.0%
cyclohexanethiol	216-378-7	1569-69-3	1569693	2054	Reach_1695	2786	2.70		2				-6.6	-6.4	-7.9	0.0%	0.0%	0.0%
bromoethane	600-588-4	104617-50-7	104617507	5593	Reach_4069	2787							-6.7	-6.4	-8.4	0.0%	0.0%	0.0%
1-methylnaphthalene	201-966-8	90-12-0	90120	1000	Reach_359	2788	3.72	0.70	16	2.72	0.70		-6.6	-6.4	-7.6	0.0%	0.0%	0.0%
2,6,10-Trimethyldodecane	622-542-2	3891-98-3	3891983	2829	Reach_4576	2789	1.33	0.38	3	1.81			-6.5	-6.4	-8.3	0.0%	0.0%	0.0%
butane-2,3-diol	208-173-6	513-85-9	513859	3038	Reach_1318	2790	6.24	1.04	3	5.24	1.04		-6.2	-6.4	-8.0	0.0%	0.0%	0.0%
furan	202-458-9	95-85-2	95852	4136	Reach_445	2791	3.52	0.48	3				-6.7	-6.4	-8.4	0.0%	0.0%	0.0%
hexachloroacetone	217-285-4	1798-60-3	1798603	2162	Reach_1721	2792	4.88	0.56	3				-6.7	-6.4	-8.3	0.0%	0.0%	0.0%
2,4-dichloro-α,α,α-trifluorotoluene	610-122-1	433733-94-9	433733949	2910	Reach_4321	2793	4.68	2.07	3				-6.7	-6.4	-8.6	0.0%	0.0%	0.0%
4-methyl-N-[3-(4-methyl-1H-imidazol-1-yl)-5-(trifluoromethyl)ph	613-879-6	66069-32-7	66069327	5977	Reach_4388	2794							-5.8	-6.4	-7.9	0.0%	0.0%	0.0%
615-790-8	615-790-8	72714-62-6	72714626	3610	Reach_4417	2795	1.78	2.33	3				-6.6	-6.4	-8.6	0.0%	0.0%	0.0%
heptan-2-one	203-767-1	110-43-0	110430	278	Reach_814	2796	5.06	0.12	3	4.37	0.21		-6.6	-6.4	-7.8	0.0%	0.0%	0.0%
2,3,4,5-tetrafluorobenzoyl chloride	610-950-3	53056-20-5	53056205	3085	Reach_4340	2797	3.69	0.29	3				-6.7	-6.4	-8.2	0.0%	0.0%	0.0%
dibutyl sebacate	203-672-5	109-43-3	109433	1500	Reach_773	2798	2.79	0.29	3				-6.5	-6.4	-7.6	0.0%	0.0%	0.0%
3,3-dimethylbutyryl chloride	201-901-3	89-36-1	89361	3972	Reach_341	2799	2.28	3.12	3				-6.7	-6.4	-8.0	0.0%	0.0%	0.0%
600-558-0	220-836-1	2915-57-3	2915573	2559	Reach_1884	2800	5.01	0.78	3	4.01	0.78		-6.6	-6.4	-7.8	0.0%	0.0%	0.0%
3-fluorotoluene	277-730-3	74124-79-1	74124791	3632	Reach_2942	2801	4.87	1.84	3				-6.7	-6.4	-8.4	0.0%	0.0%	0.0%
3-(diethoxymethylsilyl)propylamine	217-284-9	1798-50-1	1798501	5746	Reach_1720	2802	5.17		1				-6.6	-6.4	-7.9	0.0%	0.0%	0.0%
dimethylsulphamoyl chloride	801-489-0	128346-46-3	128346463	5653	Reach_5056	2803							-6.6	-6.4	-8.0	0.0%	0.0%	0.0%
methyl 3-α,7-α-diacetoxy-12-α-hydroxy-5-β-cholan-24-oate	223-151-6	3749-87-9	3749879	2800	Reach_1989	2804	5.37	0.22	3	4.37	0.22		-5.8	-6.4	-7.7	0.0%	0.0%	0.0%
1,3-diphenylpropane-1,3-dione	204-398-9	120-46-7	120467	1712	Reach_994	2805	3.79	0.32	3	2.79	0.32		-6.5	-6.4	-8.0	0.0%	0.0%	0.0%
1,2,3-trichloro-5-(trifluoromethyl)benzene	608-991-7	344348-40-9	344348409	2705	Reach_4285	2806	3.60	0.38	3				-6.7	-6.4	-8.6	0.0%	0.0%	0.0%
m-tolyl isocyanate	252-021-1	34432-92-3	34432923	2704	Reach_2677	2807	4.18		1				-6.6	-6.4	-7.6	0.0%	0.0%	0.0%
617-345-3	282-716-5	84332-87-6	84332876	6050	Reach_2971	2808	2.56		1				-5.8	-6.4	-7.9	0.0%	0.0%	0.0%
617-351-6	617-712-8	85448-44-8	85448448	6059	Reach_4473	2809							-5.8	-6.4	-7.9	0.0%	0.0%	0.0%
toluene-2-sulphonamide	201-808-8	88-19-7	88197	3951	Reach_319	2810	5.16		2	4.85			-5.9	-6.4	-8.0	0.0%	0.0%	0.0%
bis(3,5,5-trimethylhexanoyl) peroxide	223-356-0	3851-87-4	3851874	2823	Reach_1995	2811	4.35	0.37	3	3.80	0.71		-6.5	-6.4	-8.2	0.0%	0.0%	0.0%
1,4,7-triazonanetriium sulfate (2:3)	700-907-8	220493-36-7	220493367	5778	Reach_5023	2812							-6.2	-6.4	-7.8	0.0%	0.0%	0.0%
604-106-3	202-709-2	98-87-3	98873	4195	Reach_522	2813	3.56	0.96	3				-6.6	-6.4	-8.0	0.0%	0.0%	0.0%
617-344-8	278-757-3	77743-24-9	77743249	6035	Reach_2950	2814							-5.8	-6.4	-7.9	0.0%	0.0%	0.0%
2-chloro-6-fluorotoluene	688-269-6	641571-11-1	641571111	3428	Reach_4642	2815	4.12		1				-6.7	-6.4	-8.4	0.0%	0.0%	0.0%
methyl (S)-(-)-lactate	251-846-4	34140-91-5	34140915	5850	Reach_2671	2816	2.47	0.68	3	1.47	0.68		-6.6	-6.4	-8.1	0.0%	0.0%	0.0%
614-477-3	245-910-0	23847-08-7	23847087	2360	Reach_2536	2817	5.32	0.77	3	4.32	0.77		-6.6	-6.4	-7.8	0.0%	0.0%	0.0%
canrenone	603-835-4	134568-16-4	134568164	1879	Reach_4130	2818	4.75	0.53	3				-5.9	-6.4	-7.8	0.0%	0.0%	0.0%
4-bromoanisole	203-252-1	104-92-7	104927	1402	Reach_633	2819	4.29	0.12	3				-6.7	-6.4	-7.6	0.0%	0.0%	0.0%
tetrahydrofuran-3-carbaldehyde	209-193-8	558-30-5	558305	3180	Reach_1372	2820	5.24	0.32	3	4.24	0.32		-6.6	-6.4	-7.8	0.0%	0.0%	0.0%
methyl laurate	203-911-3	111-82-0	111820	1559	Reach_873	2821	3.77	1.53	3	2.88	1.66		-6.7	-6.4	-8.2	0.0%	0.0%	0.0%
610-979-1	617-351-6	82544-13-6	82544136	3832	Reach_4458	2822	2.90		1				-6.7	-6.4	-7.6	0.0%	0.0%	0.0%
1,4-bis[chloro(difluoro)methyl]benzene	800-301-4	862574-88-7	862574887	3901	Reach_5042	2823	3.73	1.18	3				-6.7	-6.4	-8.5	0.0%	0.0%	0.0%
2-methylnaphthalene	203-224-9	104-66-5	104665	1397	Reach_625	2824	3.06	0.25	3	2.06	0.25		-6.7	-6.4	-7.8	0.0%	0.0%	0.0%
1-bromopentane	211-684-7	685-88-1	685881	3520	Reach_1501	2825	1.70		1				-6.7	-6.4	-8.6	0.0%	0.0%	0.0%
disodium 6-acetamido-4-hydroxy-3-[[4-[[2-(sulphonatooxy)ethyl	243-653-9	20262-58-2	20262582	5766	Reach_2490	2826	5.04	0.78	3	4.45	0.98		-6.2	-6.4	-7.8	0.0%	0.0%	0.0%
N-(1-oxooctyl)glycine	238-122-3	14246-53-8	14246538	1956	Reach_2361	2827	5.14	0.80	3	4.14	0.80		-5.9	-6.4	-8.0	0.0%	0.0%	0.0%
2,5,7,10-tetraoxaundecane	213-554-5	976-71-6	976716	4170	Reach_1623	2828	3.84	0.38	3	2.84	0.38		-6.6	-6.4	-7.8	0.0%	0.0%	0.0%
cycloocta-1,5-diene	613-975-8	666816-98-4	666816984	3477	Reach_4392	2829	2.59	0.58	3				-6.7	-6.4	-8.4	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
dichloroacetyl chloride	201-199-9	79-36-7	79367	3772	Reach_241	2830	6.62		1				-6.8	-6.4	-8.4	0.0%	0.0%	0.0%
4-(methylthio)-m-cresol	209-842-5	594-44-5	594445	3277	Reach_1399	2831	3.12	2.91	3				-6.6	-6.4	-8.0	0.0%	0.0%	0.0%
androsta-1,4-diene-3,17-dione	212-977-2	897-06-3	897063	3983	Reach_1587	2832	4.70		1				-6.5	-6.4	-7.9	0.0%	0.0%	0.0%
4-amino-N-[4-(aminocarbonyl)phenyl]benzamide	277-874-7	74441-06-8	74441068	3636	Reach_2944	2833							-5.6	-6.4	-8.0	0.0%	0.0%	0.0%
1-bromodecane	222-423-1	3467-59-2	3467592	2712	Reach_1966	2834	5.78		1				-6.7	-6.4	-8.7	0.0%	0.0%	0.0%
2-nitrobenzaldehyde	209-025-3	552-89-6	552896	697	Reach_1360	2835	4.29		1				-6.6	-6.4	-8.0	0.0%	0.0%	0.0%
α,α,α,β,β,β-hexafluoro-m-xylene	207-300-2	460-00-4	460004	2946	Reach_1282	2836	3.72	0.18	3				-6.7	-6.5	-8.7	0.0%	0.0%	0.0%
norethisterone	603-746-0	13349-82-1	13349821	1867	Reach_4127	2837	5.07	1.00	3				-5.9	-6.5	-7.9	0.0%	0.0%	0.0%
benzylidene(methyl)amine	210-728-2	622-29-7	622297	3364	Reach_1444	2838	3.72	0.73	3				-6.7	-6.5	-7.5	0.0%	0.0%	0.0%
dichloro(methyl)(vinyl)silane	204-710-3	124-70-9	124709	1793	Reach_1082	2839	5.74	0.60	3	4.66	0.39		-6.7	-6.5	-8.7	0.0%	0.0%	0.0%
2-methoxyethyl acrylate	221-499-3	3121-61-7	3121617	2621	Reach_1919	2840	3.79	0.15	3	2.79	0.15		-6.6	-6.5	-7.8	0.0%	0.0%	0.0%
613-941-2	260-252-4	56539-66-3	56539663	3201	Reach_2816	2841	6.17	0.45	3	5.17	0.45		-6.7	-6.5	-7.9	0.0%	0.0%	0.0%
benzil	205-157-0	134-81-6	134816	1883	Reach_1128	2842	3.19	1.10	3				-6.7	-6.5	-8.0	0.0%	0.0%	0.0%
4,10-dibromodibenzo[def,mno]chrysene-6,12-dione	204-984-4	130-26-7	130267	1834	Reach_1118	2843	4.35	0.39	3	3.35	0.39		-6.3	-6.5	-7.4	0.0%	0.0%	0.0%
dodecyl methyl sulphide	241-972-8	18063-03-1	18063031	2163	Reach_2450	2844	5.26	0.29	3	4.26	0.29		-6.7	-6.5	-8.7	0.0%	0.0%	0.0%
propionyl chloride	201-170-0	79-03-8	79038	3764	Reach_224	2845	3.73	1.06	3	2.73	1.06		-6.7	-6.5	-8.2	0.0%	0.0%	0.0%
trans-1-(1-oxohexadecyl)-4-[(1-oxohexadecyl)oxy]-L-proline	255-490-0	41672-81-5	41672815	2882	Reach_2746	2846	4.69		2				-6.7	-6.5	-6.9	0.0%	0.0%	0.0%
octahydrocyclopenta[c]pyrrole	227-114-5	5661-03-0	5661030	3206	Reach_2131	2847	5.00		1				-6.7	-6.5	-8.0	0.0%	0.0%	0.0%
sodium (4,6-dimethoxypyrimidin-2-yl)({[3-(2,2,2-trifluoroethoxy)	700-684-7	80793-17-5	80793175	3798	Reach_4967	2848	3.01	0.16	3				-6.2	-6.5	-7.8	0.0%	0.0%	0.0%
612-101-2	608-356-4	2941-20-0	2941200	2564	Reach_4272	2849	3.82	0.70	3				-6.7	-6.5	-8.6	0.0%	0.0%	0.0%
N-amidinosarcosine	203-581-0	108-42-9	108429	238	Reach_744	2850	3.70	1.09	8	2.43	1.44		-5.5	-6.5	-8.2	0.0%	0.0%	0.0%
phenolphthalein	201-004-7	77-09-8	77098	879	Reach_179	2851	4.05	0.57	3	3.05	0.57		-6.0	-6.5	-7.7	0.0%	0.0%	0.0%
2-(trifluoromethyl)benzenesulfonyl chloride	205-319-0	138-24-9	138249	5684	Reach_1140	2852							-6.7	-6.5	-7.7	0.0%	0.0%	0.0%
N-[3-(trimethoxysilyl)propyl]butylamine	242-272-5	18395-30-7	18395307	2188	Reach_2461	2853	6.34	0.67	3	5.03	0.44		-6.6	-6.5	-8.2	0.0%	0.0%	0.0%
620-225-3	617-339-0	824-80-6	824806	6044	Reach_4450	2854							-6.1	-6.5	-7.7	0.0%	0.0%	0.0%
604-112-6	211-910-4	709-55-7	709557	3576	Reach_1519	2855	4.33		1				-6.7	-6.5	-8.7	0.0%	0.0%	0.0%
bromomethane	200-813-2	74-83-9	74839	837	Reach_109	2856	3.45	0.55	10	2.45	0.55		-6.8	-6.5	-8.5	0.0%	0.0%	0.0%
2-(2-butoxyethoxy)ethyl methacrylate	230-813-8	7328-22-5	7328225	3618	Reach_2238	2857	4.75	0.27	3	3.75	0.27		-6.7	-6.5	-8.0	0.0%	0.0%	0.0%
605-830-2	204-203-7	117-69-1	117691	1663	Reach_960	2858	3.87	0.69	3				-5.5	-6.5	-8.3	0.0%	0.0%	0.0%
ethyl 2-chloropropionate	202-266-5	93-67-4	93674	4077	Reach_404	2859	3.34	0.34	3				-6.7	-6.5	-7.9	0.0%	0.0%	0.0%
617-546-6	617-546-6	84170-74-1	84170741	3857	Reach_4466	2860	3.93	0.52	3	2.93	0.52		-6.7	-6.5	-8.1	0.0%	0.0%	0.0%
tetrahydrocyclopenta[c]pyrrole-1,3(2H,3aH)-dione	606-984-3	22327-32-8	22327328	2330	Reach_4231	2861	4.96	0.30	3				-5.6	-6.5	-8.3	0.0%	0.0%	0.0%
tert-butyl (6S)-6-[4-(7-bromo-9,9-difluoro-9H-fluoren-2-yl)-1H-im	204-005-0	112-77-6	112776	1603	Reach_924	2862	0.65	0.41	3				-6.0	-6.5	-7.9	0.0%	0.0%	0.0%
dibutylbis(dodecylthio)stannane	214-688-7	1185-81-5	1185815	6392	Reach_1667	2863	2.90		2				-6.2	-6.5	-7.8	0.0%	0.0%	0.0%
α,α-bis[4-(dimethylamino)phenyl]-4-(phenylamino)naphthalene-	229-851-8	6786-83-0	6786830	3502	Reach_2206	2864	4.29	0.23	3	3.29	0.23		-6.1	-6.5	-7.7	0.0%	0.0%	0.0%
diethyl phenylphosphonite	700-781-4	160332-89-8	160332898	5729	Reach_4993	2865							-6.7	-6.5	-7.6	0.0%	0.0%	0.0%
naphthalene-1,5-diol	239-350-6	15308-01-7	15308017	2030	Reach_2384	2866	2.79	0.26	3				-5.7	-6.5	-8.1	0.0%	0.0%	0.0%
acenaphthene	201-469-6	83-32-9	83329	952	Reach_281	2867	2.96	0.70	48	1.96	0.70		-6.7	-6.5	-7.5	0.0%	0.0%	0.0%
605-954-7	209-282-1	565-61-7	565617	3203	Reach_1376	2868	4.66	1.05	3				-6.7	-6.5	-8.0	0.0%	0.0%	0.0%
[4-(2-hydroxyethoxy)-1,3-phenylene]diammonium sulphate	274-713-2	70643-20-8	70643208	6005	Reach_2919	2869	4.10		2				-6.2	-6.5	-7.8	0.0%	0.0%	0.0%
617-708-6	214-371-3	1123-25-7	1123257	1582	Reach_1661	2870	5.14		1				-5.8	-6.5	-7.9	0.0%	0.0%	0.0%
2-thienylacetonitrile	227-998-2	6065-63-0	6065630	3314	Reach_2152	2871	3.12	0.81	3				-6.7	-6.5	-7.9	0.0%	0.0%	0.0%
dimethyl(propyl)amine	213-139-9	926-63-6	926636	4042	Reach_1598	2872	4.42	0.61	3	3.55	0.70		-6.7	-6.5	-7.9	0.0%	0.0%	0.0%
619-817-4	619-817-4	52671-72-4	52671724	3067	Reach_4548	2873	5.04	0.37	3				-5.9	-6.5	-8.1	0.0%	0.0%	0.0%
dodecanal	203-983-6	112-54-9	112549	333	Reach_912	2874	2.52	0.75	4	1.80	0.75		-6.7	-6.5	-8.2	0.0%	0.0%	0.0%
1,3,3-trimethyl-N-(2-methylpropylidene)-5-[(2-methylpropyliden	200-832-6	75-02-5	75025	3655	Reach_124	2875	5.13	0.43	3	4.13	0.43		-6.6	-6.5	-7.3	0.0%	0.0%	0.0%
606-356-9	617-931-9	868-84-8	868848	3912	Reach_4480	2876	3.39	1.22	3				-6.7	-6.5	-7.7	0.0%	0.0%	0.0%
3-methylpent-3-en-2-one	209-283-7	565-62-8	565628	3204	Reach_1377	2877	4.96	0.48	3				-6.7	-6.5	-7.8	0.0%	0.0%	0.0%
4,5-dimethyl-2-(propan-2-yl)phenol	255-982-5	42872-30-0	42872300	2902	Reach_2753	2878	3.71		1				-6.7	-6.5	-8.0	0.0%	0.0%	0.0%
(Z)-3-hexenyl salicylate	265-745-8	65405-77-8	65405778	3452	Reach_2872	2879	3.19	0.47	3	2.49	0.52		-6.6	-6.5	-7.9	0.0%	0.0%	0.0%
4,6-Dichloro-2-ethoxypyrimidine	282-810-6	84434-11-7	84434117	3864	Reach_2974	2880	3.40	0.68	3	2.50	0.72		-6.7	-6.5	-7.9	0.0%	0.0%	0.0%
buta-1,2-diene	209-865-0	595-37-9	595379	738	Reach_1400	2881	6.17		1				-6.8	-6.5	-8.8	0.0%	0.0%	0.0%
(1S)-1-(2,6-dichloro-3-fluorophenyl)ethanol	619-997-4	764667-65-4	764667654	3712	Reach_4555	2882	3.54	0.80	3				-6.7	-6.5	-7.7	0.0%	0.0%	0.0%
p-tolyl isocyanate	242-616-4	18835-34-2	18835342	2211	Reach_2470	2883	6.38	0.27	3	5.38	0.27		-6.7	-6.5	-7.7	0.0%	0.0%	0.0%
800-940-9	800-940-9	35836-72-7	35836727	2750	Reach_5049	2884	3.93	0.28	3	2.93	0.28		-6.7	-6.5	-8.0	0.0%	0.0%	0.0%
ethyl difluoroacetate	619-799-8	66309-83-9	66309839	3468	Reach_4546	2885	4.06		1				-6.7	-6.5	-8.1	0.0%	0.0%	0.0%
4-tert-butylcyclohexyl chloroformate	207-787-1	494-19-9	494199	2980	Reach_1295	2886	3.37	0.37	3				-6.7	-6.5	-8.7	0.0%	0.0%	0.0%
isopropyl 2-bromo-2-methylpropionate	257-158-0	51368-55-9	51368559	3037	Reach_2772	2887	4.31		2				-6.7	-6.5	-8.3	0.0%	0.0%	0.0%
(R)-3,7-dimethyloct-6-enal	203-379-2	106-26-3	106263	1433	Reach_663	2888	4.23	0.68	3	3.05	0.10		-6.7	-6.5	-7.7	0.0%	0.0%	0.0%
butan-2-one O,O',O'',O'''-silanetetrayltetraoxime	251-882-0	34206-40-1	34206401	2694	Reach_2673	2889	5.12	0.89	3	4.12	0.89		-6.7	-6.5	-6.8	0.0%	0.0%	0.0%
5-sulphoisophthalic acid	221-696-4	3195-24-2	3195242	2640	Reach_1931	2890	3.78	0.67	3				-5.6	-6.5	-8.3	0.0%	0.0%	0.0%
propane-1,2,3-triyl 2-ethylhexanoate	230-896-0	7360-38-5	7360385	3624	Reach_2241	2891	1.91	0.09	3				-6.3	-6.5	-7.0	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
1-[4-(Chlorocarbonyl)benzyl]-4- methylpiperazinediium dichlorid	220-165-4	2649-76-5	2649765	2472	Reach_1851	2892	2.46	0.71	3				-6.2	-6.5	-7.9	0.0%	0.0%	0.0%
nadide	200-184-4	53-84-9	53849	3113	Reach_21	2893	6.04	2.30	3				-5.6	-6.5	-8.1	0.0%	0.0%	0.0%
3,4-dichloro-N-(5-chloro-2-hydroxy-4-nitrophenyl)benzamide	601-327-7	114772-54-2	114772542	1625	Reach_4083	2894	2.04	0.75	3	1.45	0.71		-6.0	-6.5	-7.9	0.0%	0.0%	0.0%
isopropenyl methyl ether	604-075-6	138401-24-8	138401248	4396	Reach_4140	2895	3.36	0.16	3	2.36	0.16		-6.8	-6.5	-8.4	0.0%	0.0%	0.0%
1,3-diisopropylbenzene	202-773-1	99-62-7	99627	4210	Reach_534	2896	2.92	0.37	3	2.23	0.26		-6.7	-6.5	-8.7	0.0%	0.0%	0.0%
3,3,10,10-tetramethoxy-2,11-dioxa-3,10-disiladodecane	617-969-6	87135-01-1	87135011	3918	Reach_4482	2897	3.67	0.53	3				-6.7	-6.5	-8.0	0.0%	0.0%	0.0%
dodecyl acrylate	218-463-4	2156-97-0	2156970	533	Reach_1765	2898	4.60	0.92	3	3.32	1.01		-6.7	-6.5	-8.5	0.0%	0.0%	0.0%
sodium 8-phenylamino-5-(4-(3-sulphonatophenylazo)-1-naphthy	600-553-3	10429-07-9	10429079	1389	Reach_4067	2899	2.82	0.24	3				-6.2	-6.5	-7.9	0.0%	0.0%	0.0%
4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol	209-218-2	561-41-1	561411	3187	Reach_1373	2900	4.26	0.27	3	2.79	0.41		-5.9	-6.5	-8.0	0.0%	0.0%	0.0%
N-(4-amino-5-chloro-2-hydroxyphenyl)-3,4-dichlorobenzamide	600-198-4	101377-47-3	101377473	1319	Reach_4057	2901	4.03		2				-6.0	-6.5	-8.3	0.0%	0.0%	0.0%
betamethasone	206-825-4	378-44-9	378449	619	Reach_1261	2902	4.96	0.48	3				-6.1	-6.5	-7.7	0.0%	0.0%	0.0%
trichloroisobutylsilane	242-053-4	18169-57-8	18169578	2171	Reach_2454	2903	6.34	0.67	3	5.03	0.44		-6.7	-6.5	-8.1	0.0%	0.0%	0.0%
isopentyl p-methoxycinnamate	275-702-5	71617-10-2	71617102	3587	Reach_2929	2904	3.70	1.90	3	2.82	1.74		-6.7	-6.5	-7.9	0.0%	0.0%	0.0%
tert-pentyl hydroperoxide	222-321-7	3425-61-4	3425614	2698	Reach_1959	2905	3.52		2				-6.7	-6.5	-7.7	0.0%	0.0%	0.0%
di-tert-butyl 3,3,5-trimethylcyclohexylidene diperoxide	229-782-3	6731-36-8	6731368	3488	Reach_2205	2906	2.81	0.49	3	1.81	0.49		-6.6	-6.5	-8.4	0.0%	0.0%	0.0%
octamethyltrisiloxane	203-497-4	107-51-7	107517	1464	Reach_710	2907	1.69	0.19	3	0.69	0.19		-6.8	-6.5	-8.6	0.0%	0.0%	0.0%
2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclotetrasiloxane	219-863-1	2554-06-5	2554065	1252	Reach_1839	2908	4.01	1.72	3	2.11	1.63		-6.4	-6.5	-8.2	0.0%	0.0%	0.0%
trimethoxy(2,4,4-trimethylpentyl)silane	251-995-5	34396-03-7	34396037	2702	Reach_2676	2909	4.94	0.83	3	3.94	0.83		-6.7	-6.5	-7.9	0.0%	0.0%	0.0%
estradiol	200-023-8	50-28-2	50282	55	Reach_7	2910	1.36	1.61	15	-0.26	1.29		-6.1	-6.5	-7.7	0.0%	0.0%	0.0%
4-amino-2,5-dichloro-N,N-dimethylbenzenesulphonamide	606-682-1	2098-65-9	2098659	2281	Reach_4212	2911	2.17	0.16	3				-5.7	-6.5	-8.1	0.0%	0.0%	0.0%
1-[(2,4-dinitrophenyl)azo]-2-naphthol	222-429-4	3468-63-1	3468631	2713	Reach_1967	2912	3.20	0.86	3				-6.1	-6.5	-8.0	0.0%	0.0%	0.0%
disodium 7-benzamido-4-hydroxy-3-[[4-[(4-sulphonatophenyl)az	220-028-9	2610-11-9	2610119	1182	Reach_1845	2913	5.26		1				-6.3	-6.5	-7.9	0.0%	0.0%	0.0%
617-834-1	696-107-0	930086-71-8	930086718	6084	Reach_4705	2914							-6.3	-6.5	-8.0	0.0%	0.0%	0.0%
dimethyl 2-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]	252-650-1	35636-63-6	35636636	2742	Reach_2692	2915	4.17	1.01	3	3.17	1.01		-5.8	-6.5	-8.2	0.0%	0.0%	0.0%
tert-butyl 3,5,5-trimethylperoxyhexanoate	236-050-7	13122-18-4	13122184	1847	Reach_2323	2916	3.06	0.80	3	2.06	0.80		-6.8	-6.5	-8.8	0.0%	0.0%	0.0%
trimethyl phosphonoacetate	227-663-0	5927-18-4	5927184	3272	Reach_2145	2917	3.00	3.27	3				-6.6	-6.5	-8.2	0.0%	0.0%	0.0%
cyclohexene	203-807-8	110-83-8	110838	286	Reach_831	2918	3.90	0.74	6	2.90	0.74		-6.8	-6.5	-8.7	0.0%	0.0%	0.0%
N,N-dimethylisopropylamine	213-635-5	996-35-0	996350	4211	Reach_1629	2919	4.06	0.69	3	3.22	0.84		-6.7	-6.5	-7.9	0.0%	0.0%	0.0%
3,3'-dimethylbiphenyl-4,4'-diyl diisocyanate	202-112-7	91-97-4	91974	4025	Reach_382	2920	3.60	0.50	3	2.60	0.50		-6.6	-6.5	-7.9	0.0%	0.0%	0.0%
3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctan-1-ol	211-477-1	647-42-7	647427	3443	Reach_1485	2921	3.85	0.16	3	2.78	0.22		-6.8	-6.5	-9.2	0.0%	0.0%	0.0%
methyl (R)-lactate	241-420-6	17392-83-5	17392835	2134	Reach_2432	2922	5.94	0.47	3	4.94	0.47		-6.7	-6.5	-8.1	0.0%	0.0%	0.0%
methyl bromoacetate	202-499-2	96-32-2	96322	4144	Reach_461	2923	4.72	1.96	3				-6.7	-6.5	-8.0	0.0%	0.0%	0.0%
N,N'-(3,3'-dimethylbiphenyl-4,4'-ylene)di(acetoacetamide)	202-111-1	91-96-3	91963	4024	Reach_381	2924	3.41	0.65	3				-5.9	-6.5	-8.2	0.0%	0.0%	0.0%
2-aminophenol	202-431-1	95-55-6	95556	4127	Reach_434	2925	3.53	0.70	3				-5.7	-6.5	-8.2	0.0%	0.0%	0.0%
trisodium 1-(1-naphthylazo)-2-hydroxynaphthalene-4',6,8-trisulp	220-036-2	2611-82-7	2611827	5803	Reach_1846	2926							-6.3	-6.5	-7.9	0.0%	0.0%	0.0%
2-[4-(4-ethoxyphenyl)-6-phenyl-1,3,5-triazin-2-yl]phenol	700-875-5	1195231-94-7	1195231947	1693	Reach_5017	2927	2.88		2				-6.1	-6.5	-8.1	0.0%	0.0%	0.0%
allyl 3-cyclohexylpropionate	220-292-5	2705-87-5	2705875	2493	Reach_1857	2928	3.09	0.50	3	2.10	0.53		-6.7	-6.5	-7.7	0.0%	0.0%	0.0%
7-anilino-4-hydroxynaphthalene-2-sulphonic acid	219-031-8	2321-07-5	2321075	1245	Reach_1784	2929	3.69	0.37	3				-5.7	-6.5	-8.1	0.0%	0.0%	0.0%
isobutyl 5-chloro-2,2-dimethylpentanoate	620-343-5	51336-94-8	51336948	3034	Reach_4566	2930	2.60		1				-6.8	-6.5	-8.2	0.0%	0.0%	0.0%
N-(2-ethylhexyl)naphthalen-2-amine	700-328-0	776-04-5	776045	3733	Reach_4862	2931	4.39	0.42	3				-6.5	-6.5	-8.2	0.0%	0.0%	0.0%
619-692-6	219-674-4	2495-37-6	2495376	565	Reach_1822	2932	3.55	0.29	3	2.55	0.29		-5.9	-6.5	-8.0	0.0%	0.0%	0.0%
dihexyl adipate	203-757-7	110-33-8	110338	1518	Reach_811	2933	2.71		2				-6.6	-6.5	-7.7	0.0%	0.0%	0.0%
trifluoromethane	200-872-4	75-46-7	75467	3674	Reach_146	2934	5.50	0.31	3	4.50	0.31		-7.0	-6.5	-8.8	0.0%	0.0%	0.0%
dibutyl 2,2'-thiobisacetate	223-914-3	4121-12-4	4121124	1264	Reach_2014	2935	3.93	0.71	3				-6.7	-6.5	-8.1	0.0%	0.0%	0.0%
3,3'-(1,4-Phenylene)bis(5,6-diphenyl-1,2,4-triazine)	258-221-5	52846-56-7	52846567	3078	Reach_2789	2936	4.17	1.01	3	3.17	1.01		-6.1	-6.5	-7.6	0.0%	0.0%	0.0%
N-{(1R)-1-cyano-2-[5-cyano-2-(trifluoromethyl)phenoxy]-1-meth	600-753-0	106483-59-4	106483594	1436	Reach_4074	2937	3.81	0.60	3				-5.9	-6.5	-7.9	0.0%	0.0%	0.0%
605-546-9	209-080-3	555-06-6	555066	5932	Reach_1364	2938							-6.7	-6.5	-8.0	0.0%	0.0%	0.0%
1,3-Benzenediamine, coupled with diazotized m-phenylenediam	282-617-7	84281-74-3	84281743	3859	Reach_2970	2939	3.72	0.71	3	2.72	0.71		-5.9	-6.5	-8.1	0.0%	0.0%	0.0%
ethyl 2,3-epoxy-3-phenylbutyrate	201-061-8	77-83-8	77838	3738	Reach_186	2940	4.35	0.52	3	3.63	0.46		-6.7	-6.5	-8.1	0.0%	0.0%	0.0%
1,2,3,4-tetrahydroisoquinoline	202-050-0	91-21-4	91214	4014	Reach_373	2941	4.41		1				-6.8	-6.5	-7.7	0.0%	0.0%	0.0%
N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2,5-di	235-426-8	12225-08-0	12225080	1744	Reach_2304	2942	4.17	1.05	3	3.17	1.05		-6.1	-6.5	-8.1	0.0%	0.0%	0.0%
hexanal	618-251-5	89182-60-5	89182605	3969	Reach_4489	2943	5.15	0.61	3	4.15	0.61		-6.8	-6.5	-8.0	0.0%	0.0%	0.0%
undecanal	203-972-6	112-44-7	112447	1589	Reach_907	2944	3.58	0.27	3	2.58	0.27		-6.8	-6.5	-8.1	0.0%	0.0%	0.0%
2-(2-heptadec-8-enyl-2-imidazolin-1-yl)ethanol	202-414-9	95-38-5	95385	4126	Reach_427	2945	2.26	0.46	3	1.26	0.46		-6.1	-6.5	-7.3	0.0%	0.0%	0.0%
tert-pentylbenzene	218-076-0	2049-95-8	2049958	2268	Reach_1751	2946	3.45		2				-6.8	-6.5	-8.6	0.0%	0.0%	0.0%
cyclopentylamine	213-697-3	1003-03-8	1003038	1298	Reach_1632	2947	4.92	0.24	3	4.09	0.31		-6.8	-6.6	-7.7	0.0%	0.0%	0.0%
1-o-tolylbiguanide	202-268-6	93-69-6	93696	4079	Reach_406	2948	4.58	0.51	3	3.58	0.51		-5.8	-6.6	-8.3	0.0%	0.0%	0.0%
2-methylaziridine	200-878-7	75-55-8	75558	3676	Reach_150	2949	3.48	0.46	3				-6.7	-6.6	-7.8	0.0%	0.0%	0.0%
N-(3-{[5-(4-chlorophenyl)-1-(2,6-dichlorobenzoyl)-1H-pyrrolo[2,3	700-829-4	5324-06-1	5324061	1273	Reach_5003	2950	6.28	0.84	3				-6.4	-6.6	-7.9	0.0%	0.0%	0.0%
trifluoromethanesulphonic acid	216-087-5	1493-13-6	1493136	2005	Reach_1687	2951	5.09	0.72	3	4.09	0.72		-5.7	-6.6	-8.1	0.0%	0.0%	0.0%
dimethoxydimethylsilane	214-189-4	1112-39-6	1112396	1544	Reach_1647	2952	5.73	0.60	3	4.40	0.54		-6.8	-6.6	-8.5	0.0%	0.0%	0.0%
methyl 3-α,7-α-diacetoxy-12-oxo-5-β-cholan-24-oate	615-497-5	71809-65-9	71809659	6010	Reach_4415	2953							-6.1	-6.6	-7.8	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
[nitrilotris(methylene)]trisphosphonic acid, potassium salt	279-900-2	82104-74-3	82104743	3817	Reach_2962	2954	4.36	0.93	3				-6.3	-6.6	-7.9	0.0%	0.0%	0.0%
diisopropyl adipate	230-072-0	6938-94-9	6938949	3541	Reach_2213	2955	4.06	0.39	3	3.06	0.39		-6.8	-6.6	-8.0	0.0%	0.0%	0.0%
4,4'-cyclohexylidenedi-o-cresol	237-163-4	13676-54-5	13676545	1901	Reach_2344	2956	2.60		3	1.60			-6.2	-6.6	-7.8	0.0%	0.0%	0.0%
Potassium (2S)-4-carboxy-2-(tetradecanoylamino)butanoate	700-277-4	2827-56-7	2827567	5816	Reach_4837	2957							-6.3	-6.6	-7.9	0.0%	0.0%	0.0%
N4-[3-(1H-imidazol-1-yl)propyl]-2-methylbenzene-1,4-diamine tr	700-408-5	103429-90-9	103429909	1366	Reach_4890	2958	4.90		1				-6.3	-6.6	-7.9	0.0%	0.0%	0.0%
11-piperazin-1-yldibenzo[b,f][1,4]thiazepine dihydrochloride	700-144-0	13115-71-4	13115714	1846	Reach_4780	2959	6.41	1.30	3				-6.3	-6.6	-7.9	0.0%	0.0%	0.0%
sec-butyl chloroformate	620-313-1	877179-03-8	877179038	3938	Reach_4564	2960	3.56		1				-6.8	-6.6	-8.5	0.0%	0.0%	0.0%
1-ethyl-1H-imidazol-3-ium trifluoromethanesulfonate	700-183-3	52299-25-9	52299259	3057	Reach_4796	2961							-6.3	-6.6	-7.9	0.0%	0.0%	0.0%
3-amino-4-methoxybenzanilide	204-388-4	120-35-4	120354	1710	Reach_992	2962	4.15	0.44	3				-6.0	-6.6	-8.2	0.0%	0.0%	0.0%
calcium dilactate	700-276-9	111974-74-4	111974744	5609	Reach_4836	2963							-6.3	-6.6	-7.9	0.0%	0.0%	0.0%
(3-aminophenyl)uronium chloride	700-345-3	515851-08-8	515851088	5907	Reach_4870	2964	2.98		2				-6.3	-6.6	-7.9	0.0%	0.0%	0.0%
1,1,3,3-tetramethyl-1,3-divinyldisiloxane	220-099-6	2627-95-4	2627954	2462	Reach_1849	2965	2.66	0.23	3	1.66	0.23		-6.8	-6.6	-9.0	0.0%	0.0%	0.0%
Sodium 4-fluorobenzene sulfinate	806-798-4	1262985-23-8	1262985238	1803	Reach_5081	2966	1.05	0.56	3				-6.3	-6.6	-7.9	0.0%	0.0%	0.0%
1-aminoimidazolidine-2,4-dione hydrochloride	700-027-4	17247-58-4	17247584	2127	Reach_4730	2967	4.65	0.25	3				-6.3	-6.6	-7.9	0.0%	0.0%	0.0%
1,3-propanesultone	214-317-9	1120-71-4	1120714	1572	Reach_1660	2968	5.24	0.67	3	4.07	0.33		-6.7	-6.6	-8.2	0.0%	0.0%	0.0%
605-260-4	605-260-4	161599-46-8	161599468	2080	Reach_4171	2969	4.89	1.72	3				-5.6	-6.6	-8.2	0.0%	0.0%	0.0%
1-[1,6-dimethyl-4-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]ethai	260-772-1	57499-57-7	57499577	3231	Reach_2825	2970	3.32	0.12	3				-6.7	-6.6	-7.8	0.0%	0.0%	0.0%
N-(5-chloro-2-methoxyphenyl)-2-[(2-methoxy-4-nitrophenyl)azo	240-131-2	15993-42-7	15993427	2069	Reach_2407	2971	4.43	0.90	3	3.43	0.90		-6.2	-6.6	-8.1	0.0%	0.0%	0.0%
2-methylbutyric acid	612-179-8	61597-98-6	61597986	3340	Reach_4372	2972	4.25	0.69	3	3.32	0.86		-6.4	-6.6	-8.2	0.0%	0.0%	0.0%
6-hydroxy-2-naphthoic acid	240-759-7	16712-64-4	16712644	2111	Reach_2428	2973	5.74	0.74	3	3.71	0.36		-6.0	-6.6	-8.3	0.0%	0.0%	0.0%
amitriptyline	226-971-2	5580-58-5	5580585	3179	Reach_2127	2974	5.37	0.23	3	4.37	0.23		-6.6	-6.6	-7.5	0.0%	0.0%	0.0%
2-(1-methylethoxy)ethyl acetate	242-901-3	19234-20-9	19234209	2228	Reach_2476	2975	5.38	0.21	3	4.38	0.21		-6.8	-6.6	-7.8	0.0%	0.0%	0.0%
ethylene dimethacrylate	202-617-2	97-90-5	97905	4175	Reach_491	2976	4.39	0.23	3	3.29	0.54		-6.8	-6.6	-9.0	0.0%	0.0%	0.0%
3-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexan-1-ol	254-384-1	39255-32-8	39255328	2837	Reach_2724	2977	3.73	0.63	3	3.11			-6.6	-6.6	-7.9	0.0%	0.0%	0.0%
2-chloro-N-mesitylacetamide	202-892-9	100-83-4	100834	138	Reach_570	2978	5.00		5	4.00			-5.9	-6.6	-8.1	0.0%	0.0%	0.0%
methyl 3,3-dimethylpent-4-enoate	264-431-8	63721-05-1	63721051	3417	Reach_2862	2979	4.01	0.83	3				-6.8	-6.6	-8.1	0.0%	0.0%	0.0%
dichloro(3-chloropropyl)methylsilane	232-136-3	7787-93-1	7787931	3741	Reach_2276	2980	5.25	0.61	3	4.19	0.61		-6.8	-6.6	-8.2	0.0%	0.0%	0.0%
2-methylundecanal	203-765-0	110-41-8	110418	1519	Reach_812	2981	2.33	0.23	3	1.36	0.14		-6.8	-6.6	-8.8	0.0%	0.0%	0.0%
5,7-Dimethoxy[1,2,4]triazolo[1,5-a]pyrimidin-2-amine	603-562-0	13223-43-3	13223433	1856	Reach_4124	2982	4.25	1.14	3				-6.0	-6.6	-8.2	0.0%	0.0%	0.0%
2-[(E)-(2-methoxy-5-nitrophenyl)diazenyl]-N-(2-methoxyphenyl)	228-788-3	6358-87-8	6358878	3411	Reach_2172	2983	1.27	0.48	3	3.00			-5.9	-6.6	-8.0	0.0%	0.0%	0.0%
2-ethoxy-6-hydroxypyrimidin-4(1H)-one	692-762-1	166524-65-8	166524658	2105	Reach_4679	2984	3.88	0.44	3	2.88	0.44		-5.5	-6.6	-8.3	0.0%	0.0%	0.0%
1-phenylethyl acetate	616-466-9	77501-63-4	77501634	882	Reach_4440	2985	2.33	0.93	5	0.72	0.59		-6.8	-6.6	-7.8	0.0%	0.0%	0.0%
D-α-methylbenzylamine	618-153-2	88374-05-4	88374054	3955	Reach_4488	2986	3.20	0.48	3	2.38	0.60		-6.8	-6.6	-7.7	0.0%	0.0%	0.0%
L-α-methylbenzylamine	639-778-7	887148-70-1	887148701	3963	Reach_4606	2987	2.25	0.17	3				-6.8	-6.6	-7.7	0.0%	0.0%	0.0%
2-amino-5-bromopyridin-3-ol	601-411-3	116091-63-5	116091635	1643	Reach_4087	2988	4.85	1.43	3				-5.8	-6.6	-8.1	0.0%	0.0%	0.0%
3,3'-iminodi(propylamine)	610-954-5	53075-09-5	53075095	5919	Reach_4341	2989	4.68	0.35	3	3.68	0.35		-6.2	-6.6	-8.4	0.0%	0.0%	0.0%
ethyl 2-methyl-1,3-dioxolane-2-acetate	218-145-5	2052-25-7	2052257	5769	Reach_1754	2990	2.66		1				-6.8	-6.6	-8.2	0.0%	0.0%	0.0%
androstanolone	700-599-5	54761-87-4	54761874	690	Reach_4946	2991	3.77	0.89	3				-6.2	-6.6	-7.9	0.0%	0.0%	0.0%
5-nitrofurfurylidene di(acetate)	202-166-1	92-55-7	92557	4040	Reach_387	2992	4.76	1.09	3				-6.5	-6.6	-8.2	0.0%	0.0%	0.0%
2,2-dimethyl-1,3-dioxane-4,6-dione	217-992-8	2033-24-1	2033241	2261	Reach_1747	2993	4.64	1.12	3				-6.0	-6.6	-8.1	0.0%	0.0%	0.0%
618-153-2	940-185-3	32860-09-6	32860096	2664	Reach_5166	2994	3.55	0.17	3				-6.8	-6.6	-8.0	0.0%	0.0%	0.0%
N-methyl-1-(methylthio)-2-nitrovinylamine	619-739-0	874208-98-7	874208987	3933	Reach_4540	2995	3.84	0.67	3				-6.4	-6.6	-8.1	0.0%	0.0%	0.0%
3-nitro-p-toluic acid	612-185-0	61636-08-6	61636086	3344	Reach_4374	2996	4.57		1	4.18			-6.0	-6.6	-8.3	0.0%	0.0%	0.0%
619-997-4	617-385-1	82784-24-5	82784245	6045	Reach_4459	2997							-6.0	-6.6	-8.2	0.0%	0.0%	0.0%
8-benzyl-8-azabicyclo[3.2.1]octan-3-one oxime	607-884-2	261953-36-0	261953360	2458	Reach_4251	2998	1.88	2.82	3				-5.9	-6.6	-8.2	0.0%	0.0%	0.0%
1-(allyloxy)-2-methyl-1-oxopropan-2-yl 5-amino-2-chlorobenzoat	696-318-8	174489-43-1	174489431	2137	Reach_4714	2999	3.80	0.83	3	2.80	0.83		-6.2	-6.6	-8.2	0.0%	0.0%	0.0%
(hydroxyethyl)urea	215-304-0	1320-51-0	1320510	1853	Reach_1676	3000	5.09	1.71	3	4.54			-5.5	-6.6	-8.3	0.0%	0.0%	0.0%
o-(1-methylheptyl)phenol	242-459-1	18626-98-7	18626987	2201	Reach_2466	3001	2.58	0.32	3				-6.8	-6.6	-7.6	0.0%	0.0%	0.0%
methyl (3-hydroxyphenyl)-carbamate	207-434-1	471-01-2	471012	2962	Reach_1288	3002	5.26		2				-6.2	-6.6	-8.3	0.0%	0.0%	0.0%
4,4'-oxydianiline	202-977-0	101-80-4	101804	1329	Reach_583	3003	3.79	0.73	3	2.79	0.73		-6.0	-6.6	-8.2	0.0%	0.0%	0.0%
dimethyl (2-acetoxyethyl)phosphonate	604-710-7	149934-21-4	149934214	5708	Reach_4160	3004							-6.6	-6.6	-8.3	0.0%	0.0%	0.0%
trans-N,N,N',N'-Tetrakis(2-hydroxyethyl)cyclohexane-1,4-dicarb	243-848-9	20485-39-6	20485396	2266	Reach_2494	3005	5.52		1				-5.5	-6.6	-8.3	0.0%	0.0%	0.0%
606-114-2	255-980-4	42872-29-7	42872297	2901	Reach_2752	3006	4.85		1				-6.8	-6.6	-7.7	0.0%	0.0%	0.0%
1-bromo-2-methylpropane	619-905-2	915416-45-4	915416454	4018	Reach_4553	3007	3.27		1				-6.9	-6.6	-9.0	0.0%	0.0%	0.0%
N-ethylpropylamine	243-573-4	20193-20-8	20193208	2253	Reach_2489	3008	5.20	0.92	3	4.20	0.92		-6.8	-6.6	-8.1	0.0%	0.0%	0.0%
2,5-di-tert-pentylhydroquinone	201-222-2	79-74-3	79743	3781	Reach_248	3009	2.64	0.89	3	1.64	0.89		-6.3	-6.6	-7.9	0.0%	0.0%	0.0%
1,1',1''-[methylidynetris(oxy)]trispropane	210-704-1	621-76-1	621761	3363	Reach_1443	3010	4.22	0.33	3				-6.8	-6.6	-8.1	0.0%	0.0%	0.0%
iodotrimethylsilane	240-171-0	16029-98-4	16029984	2073	Reach_2408	3011	4.83	0.27	3				-7.0	-6.6	-8.7	0.0%	0.0%	0.0%
(pentabromophenyl)methyl acrylate	261-767-7	59447-55-1	59447551	3278	Reach_2836	3012	1.78	0.78	3	0.78	0.78		-6.6	-6.6	-7.9	0.0%	0.0%	0.0%
ammonium difluoro[1,1,2,2-tetrafluoro-2-(pentafluoroethoxy)et	610-992-2	53378-52-2	53378522	5921	Reach_4344	3013	5.00	0.42	3	4.00	0.42		-6.4	-6.6	-8.0	0.0%	0.0%	0.0%
ethyl 3-[[bis(1-methylethoxy)phosphinothioyl]thio]propionate	275-965-6	71735-74-5	71735745	3588	Reach_2930	3014	4.33	0.44	3	4.04	0.17		-6.8	-6.6	-8.1	0.0%	0.0%	0.0%
Sodium O,O-diisobutyl phosphorothioate	700-323-3	908020-52-0	908020520	6080	Reach_4860	3015							-6.4	-6.6	-8.0	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
N'-(3-aminopropyl)-N,N-dimethylpropane-1,3-diamine	234-148-4	10563-29-8	10563298	1418	Reach_2298	3016	4.59	0.61	3	3.59	0.61		-6.2	-6.6	-8.4	0.0%	0.0%	0.0%
pentobarbital	700-355-8	42036-65-7	42036657	5884	Reach_4873	3017							-6.1	-6.6	-8.0	0.0%	0.0%	0.0%
1,2,3,5,6,7-hexahydro-1,1,2,3,3-pentamethyl-4H-inden-4-one	251-649-3	33704-61-9	33704619	2684	Reach_2669	3018	3.65	0.35	3	2.65	0.35		-6.8	-6.6	-7.9	0.0%	0.0%	0.0%
tert-butyl [2-({[1-methyl-5-(tritylamino)-1H-pyrazol-4-yl]carbam	200-350-6	57-83-0	57830	65	Reach_43	3019	3.78	0.08	3				-6.3	-6.6	-8.1	0.0%	0.0%	0.0%
tris(p-isocyanatophenyl) thiophosphate	223-981-9	4151-51-3	4151513	2880	Reach_2016	3020	5.50		3	4.50			-6.2	-6.6	-7.2	0.0%	0.0%	0.0%
N-[3-(dimethylamino)propyl]acrylamide	619-422-7	99305-42-7	99305427	4202	Reach_4520	3021	5.46		1				-6.1	-6.6	-8.3	0.0%	0.0%	0.0%
flucytosine	204-522-1	122-09-8	122098	1742	Reach_1026	3022	3.70	0.72	3				-5.8	-6.6	-8.2	0.0%	0.0%	0.0%
2-methoxyethyl cyanoacetate	611-267-3	554-52-9	554529	3170	Reach_4355	3023	3.62	0.58	3				-6.8	-6.6	-8.3	0.0%	0.0%	0.0%
3-(dodecylamino)propiononitrile	606-114-2	187592-70-7	187592707	2207	Reach_4194	3024	3.55	0.63	3				-6.8	-6.6	-8.0	0.0%	0.0%	0.0%
3-dimethylaminopropan-1-ol	226-970-7	5580-57-4	5580574	3178	Reach_2126	3025	5.37	0.23	3	4.37	0.23		-6.7	-6.6	-8.2	0.0%	0.0%	0.0%
1,1-dimethylprop-3-ynylamine	221-029-7	2978-58-7	2978587	2571	Reach_1893	3026	4.19	1.10	3				-6.8	-6.6	-7.9	0.0%	0.0%	0.0%
cyclopropyl methyl ketone	212-146-4	765-43-5	765435	3717	Reach_1540	3027	5.25	0.47	3				-6.8	-6.6	-7.8	0.0%	0.0%	0.0%
609-205-5	251-347-1	33021-02-2	33021022	2673	Reach_2667	3028	4.21		2				-6.7	-6.6	-8.0	0.0%	0.0%	0.0%
vinyl neononanoate	259-160-7	54423-67-5	54423675	3143	Reach_2798	3029	4.04	0.47	3	3.04	0.47		-6.9	-6.6	-8.4	0.0%	0.0%	0.0%
decyloxirane	220-667-3	2855-19-8	2855198	2537	Reach_1876	3030	2.74	0.71	3				-6.9	-6.6	-8.5	0.0%	0.0%	0.0%
oxolamine	207-096-5	434-03-7	434037	2911	Reach_1272	3031	2.70		1				-6.6	-6.6	-8.1	0.0%	0.0%	0.0%
2-methylcyclohexyl acetate	227-231-1	5726-19-2	5726192	3228	Reach_2133	3032	4.48	0.27	3	3.48	0.27		-6.8	-6.6	-8.0	0.0%	0.0%	0.0%
N,N'-ethylenedi(diacetamide)	700-469-8	187666-88-2	187666882	2208	Reach_4904	3033	4.48	1.31	3				-5.6	-6.6	-8.3	0.0%	0.0%	0.0%
2-[ethyl(4-nitrosophenyl)amino]ethyl [3-(triethoxysilyl)propyl]ca	700-840-4	160583-22-2	160583222	2075	Reach_5006	3034	3.53	0.27	3				-6.2	-6.6	-8.2	0.0%	0.0%	0.0%
N,N-dimethylhydrazine	200-316-0	57-14-7	57147	720	Reach_40	3035	4.13	0.44	10	3.13	0.44		-6.9	-6.6	-7.5	0.0%	0.0%	0.0%
tert-butyl acetate	208-760-7	540-88-5	540885	684	Reach_1336	3036	5.45	1.04	5	3.96	0.97		-6.9	-6.6	-8.3	0.0%	0.0%	0.0%
chlorodiphenylphosphine	225-059-1	4635-59-0	4635590	2951	Reach_2050	3037	4.29	1.10	3	3.99	0.88		-6.9	-6.6	-7.9	0.0%	0.0%	0.0%
1,1,3-trichloroacetone	203-963-7	112-36-7	112367	327	Reach_901	3038	6.43	0.58	5	5.43	0.58		-6.9	-6.6	-8.1	0.0%	0.0%	0.0%
2-{[(4-chloro-3-methylpyridin-2-yl)methyl]thio}-1H-benzimidazol	600-066-6	1003315-69-2	1003315692	1300	Reach_4055	3039	3.20	0.41	3				-6.2	-6.6	-8.1	0.0%	0.0%	0.0%
606-239-2	262-540-5	60958-45-4	60958454	5948	Reach_2848	3040							-5.7	-6.6	-8.3	0.0%	0.0%	0.0%
(+)-pin-2(3)-ene	232-087-8	7785-70-8	7785708	888	Reach_2274	3041	3.13	0.73	5	1.88	0.21		-6.9	-6.6	-8.8	0.0%	0.0%	0.0%
2-[(4-methyl-2-nitrophenyl)azo]-3-oxo-N-phenylbutyramide	219-730-8	2512-29-0	2512290	2416	Reach_1825	3042	4.43	0.90	3	3.43	0.90		-5.9	-6.6	-8.2	0.0%	0.0%	0.0%
methyl 2-oxopyrrolidin-1-acetate	261-926-0	59776-88-4	59776884	3287	Reach_2842	3043	3.82	2.04	3				-5.7	-6.6	-8.3	0.0%	0.0%	0.0%
2-{(R)-[(3-Methyl-4-nitropyridin-2-yl)methyl]sulfinyl}-1H-benzimi	700-088-7	6764-10-9	6764109	1285	Reach_4757	3044	3.34	0.17	3				-6.4	-6.6	-8.0	0.0%	0.0%	0.0%
sodium 4-aminonaphthalene-1-sulphonate	200-574-4	64-04-0	64040	3423	Reach_69	3045	2.81	1.27	3				-6.4	-6.6	-8.0	0.0%	0.0%	0.0%
dipotassium dihydrogen ethylenediaminetetraacetate	217-895-0	2001-94-7	2001947	5765	Reach_1743	3046	4.62		2				-6.4	-6.6	-8.0	0.0%	0.0%	0.0%
tert-butyl 4-(6-nitropyridin-3-yl)piperazine-1-carboxylate	691-244-2	106939-34-8	106939348	1450	Reach_4666	3047							-6.1	-6.6	-8.2	0.0%	0.0%	0.0%
3,5,5-trimethylhexyl acetate	261-245-9	58430-94-7	58430947	3247	Reach_2829	3048	3.90	0.46	3	2.90	0.46		-6.9	-6.6	-8.9	0.0%	0.0%	0.0%
619-738-5	207-925-0	501-53-1	501531	653	Reach_1299	3049	4.00		1				-6.8	-6.6	-8.2	0.0%	0.0%	0.0%
616-210-6	604-437-3	144690-92-6	144690926	1979	Reach_4153	3050	0.64	3.79	3				-6.2	-6.6	-7.9	0.0%	0.0%	0.0%
2-(4-fluorophenyl)-5-(5-iodo-2-methylbenzyl)thiophene	618-312-6	898566-17-1	898566171	3987	Reach_4494	3051	1.71	0.22	3				-6.2	-6.6	-7.4	0.0%	0.0%	0.0%
2-methylbutyraldehyde	203-336-8	105-83-9	105839	1420	Reach_651	3052	4.66	0.44	3	3.66	0.44		-6.9	-6.6	-7.7	0.0%	0.0%	0.0%
dibutyl methylenedithiodi(acetate)	238-289-2	14338-82-0	14338820	1965	Reach_2363	3053	4.30	0.45	3	3.30	0.45		-6.8	-6.6	-8.2	0.0%	0.0%	0.0%
dichloro(diphenyl)silane	201-251-0	80-10-4	80104	3788	Reach_258	3054	4.18	0.45	3	3.23	0.59		-6.8	-6.6	-7.9	0.0%	0.0%	0.0%
612-179-8	204-145-2	116-53-0	116530	1650	Reach_955	3055	4.81	0.10	3				-6.8	-6.6	-8.2	0.0%	0.0%	0.0%
(S)-2,2,3-trimethylcyclopent-3-ene-1-acetaldehyde	245-846-3	23727-15-3	23727153	2356	Reach_2533	3056	4.01	0.19	3				-6.9	-6.6	-7.8	0.0%	0.0%	0.0%
609-206-0	608-291-1	2890-61-1	2890611	2548	Reach_4269	3057	3.91	0.38	3				-6.7	-6.7	-8.0	0.0%	0.0%	0.0%
617-648-0	617-648-0	849727-62-4	849727624	6056	Reach_4470	3058							-6.4	-6.7	-8.0	0.0%	0.0%	0.0%
carbonohydrazide	207-837-2	497-18-7	497187	2989	Reach_1296	3059	3.89	1.04	3	2.89	1.04		-5.8	-6.7	-8.3	0.0%	0.0%	0.0%
N-(5-chloro-2-methylphenyl)-3-hydroxy-4-[[2-methoxy-5-[(phen	610-868-8	52603-48-2	52603482	3065	Reach_4337	3060	4.62		2				-6.5	-6.7	-8.0	0.0%	0.0%	0.0%
3-(trimethoxysilyl)propyl (2E,4E)-hexa-2,4-dienoate	642-902-2	163802-53-7	163802537	2089	Reach_4611	3061	3.59	0.29	3				-6.9	-6.7	-8.3	0.0%	0.0%	0.0%
Diphenylmethyl (6R,7R)-3-hydroxy-8-oxo-7-[(phenylacetyl)amin	611-177-4	54639-48-4	54639484	3150	Reach_4351	3062	3.72	0.19	3				-5.9	-6.7	-8.1	0.0%	0.0%	0.0%
615-309-1	270-027-2	68400-38-4	68400384	5996	Reach_2905	3063							-6.2	-6.7	-8.3	0.0%	0.0%	0.0%
4-isopropylbenzaldehyde	616-309-4	762240-92-6	762240926	6031	Reach_4432	3064							-6.9	-6.7	-7.8	0.0%	0.0%	0.0%
2-chloro-3-(2-chloroethyl)-1,3,2-oxazaphosphinane 2-oxide	692-156-7	1101184-94-4	1101184944	5605	Reach_4673	3065							-6.7	-6.7	-8.2	0.0%	0.0%	0.0%
benzyl [(2S)-1-[(2-aminoethyl)amino]-3-(4-ethoxyphenyl)propan	617-838-3	86357-14-4	86357144	3905	Reach_4475	3066	5.48	1.47	3				-6.4	-6.7	-8.0	0.0%	0.0%	0.0%
dimethyl 3-oxoglutarate	692-944-0	1363332-77-7	1363332777	5679	Reach_4683	3067							-6.8	-6.7	-8.3	0.0%	0.0%	0.0%
1,2,3,6,-tetrahydro-N-(2-hydroxyethyl)phthalimide	605-546-9	169280-10-8	169280108	2116	Reach_4179	3068	4.04		2				-5.6	-6.7	-8.3	0.0%	0.0%	0.0%
617-347-4	617-347-4	82543-16-6	82543166	3829	Reach_4455	3069	4.59		1				-5.9	-6.7	-8.2	0.0%	0.0%	0.0%
glutaric anhydride	203-593-6	108-55-4	108554	1485	Reach_748	3070	4.82	1.39	3				-6.2	-6.7	-8.3	0.0%	0.0%	0.0%
4-(2-aminoethyl)-2-methoxyphenol	233-597-3	10258-54-5	10258545	1346	Reach_2286	3071	5.07	1.36	3				-6.3	-6.7	-8.3	0.0%	0.0%	0.0%
chlorotrifluoroethylene	201-201-8	79-38-9	79389	3774	Reach_243	3072	5.39	0.72	3	4.39	0.72		-7.1	-6.7	-8.9	0.0%	0.0%	0.0%
2-cyano-N-[(ethylamino)carbonyl]acetamide	255-202-3	41078-06-2	41078062	2869	Reach_2734	3073	4.93	1.55	3				-5.8	-6.7	-8.3	0.0%	0.0%	0.0%
604-481-3	700-279-5	4707-49-7	4707497	2961	Reach_4838	3074	4.37	1.07	3				-6.9	-6.7	-8.0	0.0%	0.0%	0.0%
dimethyl cyclohexane-1,4-dicarboxylate	202-347-5	94-60-0	94600	4106	Reach_416	3075	4.36		1				-6.9	-6.7	-8.2	0.0%	0.0%	0.0%
p-menth-1-en-8-yl acetate	203-689-8	109-63-7	109637	1505	Reach_781	3076	4.84	0.78	3	3.68	0.90		-6.9	-6.7	-7.8	0.0%	0.0%	0.0%
608-177-1	608-177-1	282102-50-5	282102505	5815	Reach_4263	3077							-6.4	-6.7	-8.0	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-etho	208-797-9	542-05-2	542052	3134	Reach_1344	3078	6.60	1.14	3	5.60	1.14		-6.4	-6.7	-8.2	0.0%	0.0%	0.0%
[1α(E),2β]-1-(2,6,6-trimethylcyclohex-3-en-1-yl)but-2-en-1-one	275-156-8	71048-82-3	71048823	3577	Reach_2925	3079	3.37	0.34	3	2.37	0.34		-6.9	-6.7	-7.9	0.0%	0.0%	0.0%
hexyl laurate	251-932-1	34316-64-8	34316648	2700	Reach_2675	3080	5.45	0.78	3	4.45	0.78		-6.7	-6.7	-8.0	0.0%	0.0%	0.0%
17α-hydroxy-2-(hydroxymethylene)pregn-4-en-20-yn-3-one	600-715-3	106092-09-5	106092095	1428	Reach_4072	3081	4.09	0.75	3				-6.1	-6.7	-8.2	0.0%	0.0%	0.0%
609-521-3	609-205-5	361366-15-6	361366156	2758	Reach_4293	3082	3.23	0.43	3				-5.8	-6.7	-8.3	0.0%	0.0%	0.0%
methyl cinnamate	203-093-8	103-26-4	103264	1362	Reach_605	3083	3.87	0.41	3	3.07	0.48		-6.9	-6.7	-8.2	0.0%	0.0%	0.0%
strontium bis[2-chloro-5-[(2-hydroxy-1-naphthyl)azo]toluene-4-s	277-335-6	73263-40-8	73263408	6013	Reach_2938	3084	4.97	1.01	3	3.97	1.01		-6.4	-6.7	-8.0	0.0%	0.0%	0.0%
2-amino-6-{[(3S)-1-(3-methylbutanoyl)piperidin-3-yl]methoxy}be	700-511-5	1917-64-2	1917642	2225	Reach_4916	3085	3.91		1				-6.3	-6.7	-8.2	0.0%	0.0%	0.0%
ethyl 2-oxopyrrolidine-1-acetate	205-532-9	142-29-0	142290	1952	Reach_1176	3086	4.47	0.65	3				-5.8	-6.7	-8.3	0.0%	0.0%	0.0%
triethoxy(methyl)silane	255-255-2	41198-08-7	41198087	631	Reach_2738	3087	1.55	1.09	37	1.11	1.66	13	-6.9	-6.7	-8.4	0.0%	0.0%	0.0%
nonamethylenediamine	211-470-3	646-24-2	646242	3439	Reach_1483	3088	4.75	0.20	3	3.75	0.20		-6.9	-6.7	-8.0	0.0%	0.0%	0.0%
3-(hydroxymethyl)pyridinium fluoride	700-352-1	62756-44-9	62756449	5958	Reach_4872	3089							-6.4	-6.7	-8.0	0.0%	0.0%	0.0%
2-Amino-4,5-dimethyl-thiophene-3-carbonitrile	616-364-4	766-36-9	766369	3722	Reach_4435	3090	4.37	0.18	3				-6.8	-6.7	-8.2	0.0%	0.0%	0.0%
4-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexan-1-ol	201-627-4	85-73-4	85734	3897	Reach_300	3091	4.65	0.57	3	3.65	0.57		-6.7	-6.7	-8.0	0.0%	0.0%	0.0%
2,3,4,6-tetrakis-O-(2,2-dimethylpropanoyl)-α-D-glucopyranosyl b	686-241-8	81058-27-7	81058277	3800	Reach_4632	3092	2.36	1.41	3				-6.7	-6.7	-8.1	0.0%	0.0%	0.0%
citronellyl acetate	205-775-0	150-84-5	150845	2012	Reach_1206	3093	3.85	0.20	3	2.85	0.20		-6.9	-6.7	-8.2	0.0%	0.0%	0.0%
608-993-8	609-521-3	38109-77-2	38109772	2817	Reach_4304	3094	4.09	0.32	3				-6.9	-6.7	-8.1	0.0%	0.0%	0.0%
trifluoro(trifluoromethoxy)ethylene	214-703-7	1187-93-5	1187935	1678	Reach_1668	3095	4.36	1.12	3	3.36	1.12		-7.0	-6.7	-9.0	0.0%	0.0%	0.0%
2,4,6-triisopropyl-m-phenylene diisocyanate	251-908-0	34274-28-7	34274287	5851	Reach_2674	3096	5.34		2	4.48			-6.7	-6.7	-7.6	0.0%	0.0%	0.0%
dibutyl terephthalate	217-803-9	1962-75-0	1962750	525	Reach_1740	3097	2.30	0.52	3	1.30	0.52		-6.9	-6.7	-8.0	0.0%	0.0%	0.0%
1-(allyloxy)-2-methyl-1-oxopropan-2-yl 2-chloro-5-nitrobenzoate	221-423-9	3089-16-5	3089165	2614	Reach_1915	3098	5.18	0.72	3	4.18	0.72		-6.8	-6.7	-8.2	0.0%	0.0%	0.0%
pyrrolidine	204-648-7	123-75-1	123751	1774	Reach_1057	3099	4.91	0.44	3	3.91	0.44		-6.9	-6.7	-8.2	0.0%	0.0%	0.0%
ethisterone	603-010-9	124750-51-2	124750512	1794	Reach_4110	3100							-6.1	-6.7	-8.1	0.0%	0.0%	0.0%
4-phenylbutan-2-one	219-847-4	2550-26-7	2550267	2437	Reach_1838	3101	5.17	0.31	3	4.17	0.31		-6.9	-6.7	-7.8	0.0%	0.0%	0.0%
N-(3-{[5-bromo-1-(2,6-dichlorobenzoyl)-1H-pyrrolo[2,3-b]pyridin	202-765-8	99-55-8	99558	1088	Reach_530	3102	4.32	0.70	16	3.32	0.70		-6.2	-6.7	-7.7	0.0%	0.0%	0.0%
1,3-bis(trimethylsilyl)urea	242-177-9	18297-63-7	18297637	2176	Reach_2457	3103	3.20	0.41	3				-6.9	-6.7	-7.9	0.0%	0.0%	0.0%
estra-4,9-diene-3,17-dione	700-798-7	877399-00-3	877399003	3941	Reach_4997	3104	3.34	1.08	3				-6.9	-6.7	-8.2	0.0%	0.0%	0.0%
607-173-7	607-977-8	26650-09-9	26650099	2481	Reach_4256	3105	3.02	0.27	3				-6.0	-6.7	-8.3	0.0%	0.0%	0.0%
tert-butyl [(3S)-3-amino-2-oxo-2,3,4,5-tetrahydro-1H-1-benzaze	609-723-1	39590-81-3	39590813	2842	Reach_4308	3106	5.96	1.09	3				-6.1	-6.7	-8.2	0.0%	0.0%	0.0%
L-menthan-3-one	237-926-1	14073-97-3	14073973	1929	Reach_2357	3107	4.76	0.22	3	3.76	0.22		-6.9	-6.7	-7.9	0.0%	0.0%	0.0%
1,1,1,3,5,5,5-heptamethyl-3-[(trimethylsilyl)oxy]trisiloxane	241-867-7	17928-28-8	17928288	2158	Reach_2448	3108	1.38	0.41	3	0.38	0.41		-6.9	-6.7	-8.1	0.0%	0.0%	0.0%
1-(2,3-dichlorophenyl)piperazine	609-736-2	39672-75-8	39672758	2847	Reach_4311	3109	5.08	0.25	3				-6.6	-6.7	-8.0	0.0%	0.0%	0.0%
benzyl methacrylate	275-639-3	71566-54-6	71566546	3584	Reach_2927	3110	-0.92	3.41	3	4.00			-6.9	-6.7	-7.9	0.0%	0.0%	0.0%
octa-1,7-diene	218-915-0	2280-49-1	2280491	2338	Reach_1781	3111	5.70	0.35	3	4.70	0.35		-7.0	-6.7	-9.1	0.0%	0.0%	0.0%
609-734-1	601-431-2	1164-92-7	1164927	1649	Reach_4088	3112	2.41		2				-6.5	-6.7	-8.0	0.0%	0.0%	0.0%
trimethoxypropylsilane	213-926-7	1067-25-0	1067250	1445	Reach_1638	3113	6.42		3	5.42			-6.9	-6.7	-8.1	0.0%	0.0%	0.0%
diacetoxydi-tert-butoxysilane	236-112-3	13170-23-5	13170235	1851	Reach_2324	3114	5.76	0.94	3	4.75	0.56		-6.9	-6.7	-8.0	0.0%	0.0%	0.0%
3,5,6-tri-O-benzyl-D-glucofuranose	601-694-3	120279-88-1	120279881	1707	Reach_4101	3115	4.35	1.19	3				-6.1	-6.7	-8.2	0.0%	0.0%	0.0%
2-phenylpropan-2-ol	210-539-5	617-94-7	617947	3354	Reach_1437	3116	3.78	0.33	3				-6.9	-6.7	-8.3	0.0%	0.0%	0.0%
ethyl 4-methyloxazole-5-carboxylate	221-341-3	3071-32-7	3071327	2610	Reach_1911	3117	3.41	0.88	3				-6.0	-6.7	-8.4	0.0%	0.0%	0.0%
methylcyclopentadiene	247-724-5	26472-00-4	26472004	2470	Reach_2582	3118	2.77		1				-7.0	-6.7	-8.5	0.0%	0.0%	0.0%
perhydropyrimidin-2-one	615-083-4	70223-33-5	70223335	3558	Reach_4408	3119	4.04		2				-6.0	-6.7	-8.3	0.0%	0.0%	0.0%
2-(2-piperazin-1-ylethoxy)ethanol	214-275-1	1119-34-2	1119342	5608	Reach_1653	3120	6.35		2				-5.9	-6.7	-8.4	0.0%	0.0%	0.0%
phenethyl acetate	606-942-4	221615-75-4	221615754	2321	Reach_4227	3121	4.67	0.73	3				-6.9	-6.7	-8.0	0.0%	0.0%	0.0%
nandrolone	256-841-0	50910-55-9	50910559	3023	Reach_2767	3122	3.96	0.09	3				-6.1	-6.7	-8.2	0.0%	0.0%	0.0%
triethyl phosphonoacetate	212-757-6	867-13-0	867130	3910	Reach_1572	3123	4.86	1.10	3	3.86	1.10		-6.0	-6.7	-8.3	0.0%	0.0%	0.0%
benzamide oxime	200-370-5	58-22-0	58220	67	Reach_46	3124	3.10	1.66	3	2.10	1.66		-6.0	-6.7	-8.3	0.0%	0.0%	0.0%
octanenitrile	613-941-2	66546-92-7	66546927	3476	Reach_4391	3125	3.78	0.71	3				-7.0	-6.7	-8.2	0.0%	0.0%	0.0%
606-947-1	606-947-1	221640-21-7	221640217	5781	Reach_4229	3126	4.10		2				-6.5	-6.7	-8.1	0.0%	0.0%	0.0%
bis(4-tert-butylphenyl)iodonium hexafluorophosphate	620-341-4	61358-25-6	61358256	5950	Reach_4565	3127	2.97	1.18	3	2.23	1.34		-6.5	-6.7	-8.1	0.0%	0.0%	0.0%
2,4-dihydroxy-3-methylbenzoic acid	696-298-0	144690-96-0	144690960	1980	Reach_4712	3128	3.17	1.30	3				-6.1	-6.7	-8.3	0.0%	0.0%	0.0%
617-590-6	700-179-1	5128-28-9	5128289	3031	Reach_4794	3129	3.97	1.11	3				-6.2	-6.7	-8.2	0.0%	0.0%	0.0%
5-nitrosalicylic acid	218-226-5	2084-69-7	2084697	2279	Reach_1757	3130	2.22	0.19	3				-6.1	-6.7	-8.4	0.0%	0.0%	0.0%
tetradecyl chloroformate	260-330-8	56677-60-2	56677602	3208	Reach_2818	3131	3.31	1.18	3	2.31	1.18		-6.9	-6.7	-8.7	0.0%	0.0%	0.0%
2-(dimethylamino)-2-methylpropan-1-ol	268-018-3	67989-88-2	67989882	5991	Reach_2894	3132	5.46	0.72	3	4.43	0.84		-6.9	-6.7	-8.3	0.0%	0.0%	0.0%
2-[2-(2-ethoxyethoxy)ethoxy]ethyl methacrylate	254-588-0	39670-09-2	39670092	2846	Reach_2727	3133	5.54	0.51	3	4.54	0.51		-6.9	-6.7	-8.4	0.0%	0.0%	0.0%
(E)-4-Hydroxy-3-methoxybenzaldehyde oxime	606-753-7	213967-55-6	213967556	2293	Reach_4217	3134	2.80	0.24	3				-6.0	-6.7	-8.4	0.0%	0.0%	0.0%
tetra-1-naphthyl 3,3',5,5'-tetra-tert-butyl-6,6'-dimethylbiphenyl-	215-836-3	1424-00-6	1424006	1955	Reach_1679	3135	3.82	0.09	3				-6.5	-6.7	-8.1	0.0%	0.0%	0.0%
8-azabicyclo[3.2.1]octan-3-ol	261-491-7	58909-56-1	58909561	3259	Reach_2833	3136	2.61	2.86	3				-6.8	-6.7	-8.3	0.0%	0.0%	0.0%
606-984-3	694-906-9	1363332-65-3	1363332653	5678	Reach_4684	3137							-7.0	-6.7	-8.0	0.0%	0.0%	0.0%
603-981-9	203-816-7	110-93-0	110930	291	Reach_838	3138	4.99	0.70	20	3.99	0.70		-6.4	-6.7	-7.8	0.0%	0.0%	0.0%
1-chloro-2-(dichloromethyl)benzene	276-719-0	72576-80-8	72576808	3607	Reach_2937	3139	6.00	0.87	3	5.00	0.87		-7.0	-6.7	-8.3	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
8-chloro-5,6-dihydro-11H-benzo[5,6]cyclohepta[1,2-b]pyridin-11	700-173-9	1072896-13-9	1072896139	1458	Reach_4790	3140	3.49	0.79	3				-6.4	-6.7	-8.5	0.0%	0.0%	0.0%
tetrahydro-2-methylfuran	202-507-4	96-47-9	96479	4147	Reach_465	3141	5.63	0.26	3	4.63	0.26		-7.0	-6.7	-8.3	0.0%	0.0%	0.0%
DL-hexane-1,2-diol	230-029-6	6920-22-5	6920225	3534	Reach_2211	3142	4.75	1.23	3				-6.9	-6.8	-8.3	0.0%	0.0%	0.0%
2-(2,4-diaminophenoxy)ethanol dihydrochloride	266-357-1	66422-95-5	66422955	5980	Reach_2880	3143	4.10		2				-6.5	-6.8	-8.1	0.0%	0.0%	0.0%
bis(2-ethylhexyl) carbonate	238-925-9	14858-73-2	14858732	2004	Reach_2372	3144	3.33	0.26	3	2.33	0.26		-6.9	-6.8	-8.8	0.0%	0.0%	0.0%
octyl (R)-2-(4-chloro-2-methylphenoxy)propionate	266-358-7	66423-13-0	66423130	3473	Reach_2881	3145	4.23	0.88	3	3.23	0.88		-6.7	-6.8	-7.9	0.0%	0.0%	0.0%
pentaerythritol tetrakis(3-mercaptopropionate)	211-941-3	717-74-8	717748	3590	Reach_1522	3146	2.14	0.20	3				-6.1	-6.8	-8.3	0.0%	0.0%	0.0%
tetrasodium 4,4'-bis[[4-morpholino-6-(p-sulphonatoanilino)-1,3,!	249-323-0	28950-61-0	28950610	5821	Reach_2626	3147							-6.5	-6.8	-8.1	0.0%	0.0%	0.0%
hexadecane	208-878-9	544-76-3	544763	3146	Reach_1354	3148	7.67		1				-6.7	-6.8	-8.4	0.0%	0.0%	0.0%
1-ethylpiperidine	242-354-0	18472-51-0	18472510	5748	Reach_2462	3149	2.24	0.70	3	1.61	1.44		-7.0	-6.8	-7.9	0.0%	0.0%	0.0%
hydrocortisone 21-acetate	200-819-5	74-88-4	74884	839	Reach_114	3150	3.15	0.19	6	2.18	0.36		-6.0	-6.8	-8.3	0.0%	0.0%	0.0%
bis(2-ethylhexyl) 2,2'-thiobisacetate	246-131-9	24293-43-4	24293434	2384	Reach_2543	3151	2.56	0.44	3	1.56	0.44		-6.8	-6.8	-7.8	0.0%	0.0%	0.0%
(3-chloropropyl)diethoxymethylsilane	236-828-6	13501-76-3	13501763	1885	Reach_2339	3152	5.59	0.16	3	4.66	0.22		-7.0	-6.8	-8.1	0.0%	0.0%	0.0%
(Z)-3-(9-octadecenylamino)propiononitrile	200-143-0	52-51-7	52517	674	Reach_16	3153	3.32	1.04	18	3.58	0.84	3	-6.8	-6.8	-7.9	0.0%	0.0%	0.0%
ethyl 2-oxocyclohexanecarboxylate	695-198-4	151604-82-9	151604829	5710	Reach_4690	3154							-7.0	-6.8	-8.4	0.0%	0.0%	0.0%
N-(4-acetylaminophenyl)-3-hydroxynaphthalene-2-carboxamide	202-189-7	92-78-4	92784	4050	Reach_393	3155	2.86	0.04	3				-6.4	-6.8	-8.3	0.0%	0.0%	0.0%
696-244-6	696-244-6	84449-85-4	84449854	6052	Reach_4711	3156							-6.5	-6.8	-8.1	0.0%	0.0%	0.0%
2-(dibenzylamino)-1-(3,4-dihydroxyphenyl)ethanone	208-307-3	521-18-6	521186	672	Reach_1323	3157	1.77	0.53	3	0.77	0.53		-6.3	-6.8	-8.2	0.0%	0.0%	0.0%
N1,N5-Dibutyl-N2-(2-ethylhexanoyl)-L-glutamamide	700-210-9	1001161-63-2	1001161632	1292	Reach_4805	3158	-0.14	1.06	3				-6.4	-6.8	-8.3	0.0%	0.0%	0.0%
1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene	228-846-8	6362-80-7	6362807	3414	Reach_2174	3159	1.86		1				-6.9	-6.8	-8.1	0.0%	0.0%	0.0%
undec-10-enal	203-973-1	112-45-8	112458	1590	Reach_908	3160	3.21	0.46	3	2.21	0.46		-7.0	-6.8	-8.2	0.0%	0.0%	0.0%
N-[3-(dimethoxymethylsilyl)-2-methylpropyl]ethylenediamine	257-851-8	52328-05-9	52328059	5911	Reach_2780	3161	6.38		1				-6.8	-6.8	-8.4	0.0%	0.0%	0.0%
ethyl (1R,2S)-1-amino-2-vinylcyclopropanecarboxylate sulfate (2	689-958-4	1173807-85-6	1173807856	5615	Reach_4654	3162							-6.5	-6.8	-8.1	0.0%	0.0%	0.0%
608-209-4	608-209-4	284461-73-0	284461730	2531	Reach_4264	3163	2.13	1.22	3	-0.07			-6.5	-6.8	-8.3	0.0%	0.0%	0.0%
2-methylquinolin-8-ol	211-448-3	645-62-5	645625	3438	Reach_1481	3164	4.30	0.14	3	3.59	0.55		-6.5	-6.8	-8.4	0.0%	0.0%	0.0%
2,3-dimethylbut-1-ene	209-262-2	563-78-0	563780	3194	Reach_1374	3165	3.95	0.15	3				-7.0	-6.8	-9.2	0.0%	0.0%	0.0%
2-phenyl-2-imidazoline	210-361-8	613-92-3	613923	3333	Reach_1423	3166	3.76	0.27	3				-6.2	-6.8	-8.3	0.0%	0.0%	0.0%
1,2-diethoxybenzene	218-089-1	2050-46-6	2050466	2269	Reach_1752	3167	4.46		2				-7.0	-6.8	-8.0	0.0%	0.0%	0.0%
2,5,6-trimethylcyclohex-2-en-1-one	938-119-3	1398498-88-8	1398498888	5687	Reach_5148	3168							-7.0	-6.8	-8.0	0.0%	0.0%	0.0%
3-(chloromethyl)heptane	246-273-1	24461-61-8	24461618	2394	Reach_2546	3169	4.63	0.98	3				-7.0	-6.8	-9.1	0.0%	0.0%	0.0%
2-isocyanatoethyl methacrylate	250-284-7	30674-80-7	30674807	2606	Reach_2648	3170	5.42	0.18	3	4.42	0.18		-7.0	-6.8	-8.2	0.0%	0.0%	0.0%
N-(2-hydroxyethyl)-N'-{1-methyl-1-[3-(1-methylethenyl)phenyl]e	200-681-6	68-22-4	68224	800	Reach_92	3171	4.07		2				-6.2	-6.8	-8.4	0.0%	0.0%	0.0%
5-phenyl-2-(2-phenylpropan-2-yl)-2H-tetrazole	611-200-8	54811-38-0	54811380	3153	Reach_4352	3172	4.44	0.10	3				-7.0	-6.8	-8.2	0.0%	0.0%	0.0%
icosane	800-181-3	371756-75-1	371756751	5863	Reach_5038	3173	5.40	0.47	3	4.40	0.47		-6.8	-6.8	-7.7	0.0%	0.0%	0.0%
methacrylic anhydride	212-084-8	760-93-0	760930	3698	Reach_1532	3174	5.07	0.62	3	4.17	0.86		-7.0	-6.8	-8.5	0.0%	0.0%	0.0%
2-methyl-3-butenenitrile	619-738-5	87305-03-1	87305031	3924	Reach_4539	3175	3.78	0.37	3	2.99	0.22		-7.0	-6.8	-8.0	0.0%	0.0%	0.0%
2,4,6-triisopropylaniline	209-388-8	575-61-1	575611	3232	Reach_1379	3176	2.91		1				-7.0	-6.8	-8.3	0.0%	0.0%	0.0%
615-749-4	237-196-4	13683-89-1	13683891	1902	Reach_2345	3177	3.72	0.53	3				-7.0	-6.8	-8.3	0.0%	0.0%	0.0%
1-(2-Ethylbutyl)cyclohexanecarbonitrile	211-014-3	627-83-8	627838	3377	Reach_1459	3178	3.94	1.03	3	2.94	1.03		-7.0	-6.8	-8.0	0.0%	0.0%	0.0%
progesterone	700-591-1	82203-23-4	82203234	3821	Reach_4943	3179	3.94	0.64	3				-6.7	-6.8	-8.2	0.0%	0.0%	0.0%
sodium nonyl sulphate	214-002-6	1072-15-7	1072157	5602	Reach_1641	3180	5.10	0.86	3	4.10	0.86		-6.5	-6.8	-8.1	0.0%	0.0%	0.0%
hexamethyldisilane	215-911-0	1450-14-2	1450142	1983	Reach_1682	3181	2.93	0.07	3				-7.2	-6.8	-9.0	0.0%	0.0%	0.0%
3,3'-di-tert-butyl-5,5'-dimethoxybiphenyl-2,2'-diol	700-291-0	1000701-92-7	1000701927	5588	Reach_4845	3182	5.14	0.15	3	4.19	0.40		-6.5	-6.8	-7.8	0.0%	0.0%	0.0%
1,4-dimethylpiperazine	203-412-0	106-58-1	106581	1439	Reach_674	3183	5.28	0.39	3	4.28	0.39		-7.0	-6.8	-8.4	0.0%	0.0%	0.0%
4-chlorobenzhydryl alcohol	200-522-0	61-90-5	61905	3359	Reach_61	3184	6.87		2				-6.9	-6.8	-8.2	0.0%	0.0%	0.0%
2,6-difluorobenzonitrile	224-709-1	4457-71-0	4457710	2927	Reach_2039	3185	5.83	0.58	3	4.83	0.58		-7.0	-6.8	-8.1	0.0%	0.0%	0.0%
616-391-1	230-875-6	7347-25-3	7347253	6015	Reach_2240	3186							-6.4	-6.8	-7.6	0.0%	0.0%	0.0%
5-methylheptan-3-one	244-169-0	21049-70-7	21049707	5771	Reach_2502	3187	4.91	0.46	3	3.91	0.46		-7.0	-6.8	-8.4	0.0%	0.0%	0.0%
tert-butyl {(2S,3R)-3-hydroxy-4-[(2-methylpropyl)amino]-1-phen	605-203-3	160232-08-6	160232086	2072	Reach_4170	3188	3.37	0.39	3				-6.2	-6.8	-8.3	0.0%	0.0%	0.0%
1-methylcyclohexane-1-carboxylic acid	238-063-3	14206-62-3	14206623	5692	Reach_2359	3189	4.79	0.27	3	3.82	0.40		-6.7	-6.8	-8.4	0.0%	0.0%	0.0%
[[(2-ethylhexyl)oxy]methyl]oxirane	219-553-6	2461-15-6	2461156	561	Reach_1814	3190	4.78	0.92	3	4.64	1.54		-7.0	-6.8	-8.8	0.0%	0.0%	0.0%
3-Ethoxyestra-3,5-dien-17-one	801-163-8	571189-16-7	571189167	3225	Reach_5053	3191	3.78	0.85	3				-6.8	-6.8	-8.2	0.0%	0.0%	0.0%
4-vinylcyclohexene	221-209-5	3031-66-1	3031661	2591	Reach_1899	3192	5.04	1.00	3	4.04	1.00		-7.0	-6.8	-9.1	0.0%	0.0%	0.0%
3-[dimethyl(3-{[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulfo	700-769-9	76201-56-4	76201564	3704	Reach_4989	3193	4.68	0.38	3	3.68	0.38		-5.9	-6.8	-8.5	0.0%	0.0%	0.0%
methyl [(dimethoxyphosphinothioyl)thio]acetate	217-443-2	1852-17-1	1852171	2196	Reach_1727	3194	6.96	0.79	3	5.96	0.79		-7.0	-6.8	-8.4	0.0%	0.0%	0.0%
(3R,4S,5S,6R,7R,9R,10Z,11S,12R,13S,14R)-6-{[[(2S,3R,4S,6R)-4-(di	619-511-0	141573-96-8	141573968	1938	Reach_4526	3195	2.58	1.49	3				-6.8	-6.8	-8.4	0.0%	0.0%	0.0%
N-[3-(dimethylamino)propyl]dodecanamide	221-661-3	3179-80-4	3179804	2638	Reach_1930	3196	2.30		2				-6.9	-6.8	-8.3	0.0%	0.0%	0.0%
2-[(1-methylpropyl)amino]ethanol	252-471-9	35265-04-4	35265044	2726	Reach_2687	3197	4.45	0.77	3	3.45	0.77		-6.9	-6.8	-8.4	0.0%	0.0%	0.0%
isopentylamine	203-526-0	107-85-7	107857	222	Reach_715	3198	4.52	0.85	4	3.52	0.70		-7.0	-6.8	-8.1	0.0%	0.0%	0.0%
octyloxirane	219-295-4	2404-44-6	2404446	2370	Reach_1799	3199	3.28	0.56	3				-7.0	-6.8	-8.9	0.0%	0.0%	0.0%
615-077-1	259-996-2	56107-04-1	56107041	3186	Reach_2812	3200	3.49	0.07	3				-7.0	-6.8	-8.4	0.0%	0.0%	0.0%
pentasodium 3,3'-({6-[(2-sulfonatoethyl)amino]-1,3,5-triazine-2,4	700-773-0	1342795-11-2	1342795112	5671	Reach_4990	3201							-6.5	-6.8	-8.2	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
di-tert-butyl α,α,α',α'-tetramethyl-(p-phenylenedimethylene) di	220-479-1	2781-00-2	2781002	2518	Reach_1866	3202	5.88		1				-6.8	-6.8	-7.8	0.0%	0.0%	0.0%
1-(4-chlorophenyl)sulfanyl-2-nitrobenzene	609-896-3	41202-77-1	41202771	2873	Reach_4314	3203	3.42	0.62	3				-6.9	-6.8	-7.8	0.0%	0.0%	0.0%
N-{3-[(5-bromo-1H-pyrrolo[2,3-b]pyridin-3-yl)carbonyl]-2,4-diflu	687-535-9	122586-52-1	122586521	1754	Reach_4634	3204	4.08		2				-6.1	-6.8	-8.4	0.0%	0.0%	0.0%
Isononanoic acid, mixed esters with dipentaerythritol, heptanoic	282-775-7	84418-63-3	84418633	3863	Reach_2973	3205	5.83	0.58	3	4.83	0.58		-7.0	-6.8	-8.4	0.0%	0.0%	0.0%
methyl benzoylformate	203-425-1	106-70-7	106707	1444	Reach_677	3206	4.79	0.72	3	3.91	0.79		-7.0	-6.8	-8.4	0.0%	0.0%	0.0%
2-methylvaleraldehyde	213-208-3	930-02-9	930029	4054	Reach_1604	3207	4.46		1	4.00			-7.0	-6.8	-8.2	0.0%	0.0%	0.0%
9H-carbazol-4-ol	258-034-9	52602-39-8	52602398	3064	Reach_2784	3208	3.69	0.23	3				-6.3	-6.8	-8.4	0.0%	0.0%	0.0%
methyl 4-[[(2,5-dichlorophenyl)amino]carbonyl]-2-nitrobenzoate	606-050-5	18531-99-2	18531992	2197	Reach_4190	3209	2.45	0.30	3				-6.2	-6.8	-8.4	0.0%	0.0%	0.0%
N-cyclohexylcyclohexanaminium (2S)-4-fluoro-4-methyl-2-({(1S)-	613-801-0	65473-13-4	65473134	5974	Reach_4387	3210							-6.6	-6.8	-8.2	0.0%	0.0%	0.0%
3-(9-anthryl)acrylaldehyde	620-448-6	566200-79-1	566200791	3207	Reach_4568	3211	2.21	1.03	3				-6.8	-6.8	-8.3	0.0%	0.0%	0.0%
3-nitro[1,1'-biphenyl]-4-ol	700-286-3	538-09-0	538090	3110	Reach_4841	3212	4.46	0.90	3				-6.4	-6.8	-8.4	0.0%	0.0%	0.0%
4,4'-Bis(methoxymethyl)biphenyl	700-008-0	3753-18-2	3753182	2802	Reach_4723	3213	3.47		2				-7.0	-6.8	-8.2	0.0%	0.0%	0.0%
ethyl chlorothiolformate	615-077-1	70174-49-1	70174491	3556	Reach_4407	3214	3.63	0.51	3				-7.1	-6.8	-8.2	0.0%	0.0%	0.0%
3,5-diiodosalicylic acid	205-124-0	133-91-5	133915	1872	Reach_1125	3215	3.84	0.32	3	2.84	0.32		-6.3	-6.8	-8.4	0.0%	0.0%	0.0%
N-methyl-1-(1-naphthyl)methanamine hydrochloride (1:1)	700-778-8	1064076-86-3	1064076863	5599	Reach_4991	3216	4.82		2				-6.6	-6.8	-8.2	0.0%	0.0%	0.0%
(S)-1,2-epoxypropane	201-182-6	79-16-3	79163	3767	Reach_233	3217	6.25	0.21	3	5.25	0.21		-7.1	-6.8	-8.5	0.0%	0.0%	0.0%
1,1'-[methylenebis(oxy)]dibutane	219-909-0	2568-90-3	2568903	2443	Reach_1840	3218	4.49	0.36	3	3.49	0.21		-7.1	-6.8	-8.3	0.0%	0.0%	0.0%
decanoyl chloride	203-938-0	112-13-0	112130	1576	Reach_889	3219	2.74	0.47	3				-7.1	-6.8	-9.1	0.0%	0.0%	0.0%
testosterone	620-466-4	140391-39-5	140391395	1928	Reach_4573	3220							-6.3	-6.8	-8.3	0.0%	0.0%	0.0%
8-chloro-11-(1-methylpiperidin-4-yl)-6,11-dihydro-5H-benzo[5,6]	220-863-9	2921-57-5	2921575	2562	Reach_1886	3221	4.35	0.66	3				-6.3	-6.8	-8.2	0.0%	0.0%	0.0%
1,1,1-triethoxy-N,N-diethylsilanamine	700-051-5	35077-00-0	35077000	2721	Reach_4740	3222	4.78		2				-5.9	-6.8	-8.5	0.0%	0.0%	0.0%
1,1'-(1,1,2,2-tetramethylethylene)dibenzene	217-568-2	1889-67-4	1889674	2214	Reach_1732	3223	6.22	0.24	3	5.22	0.24		-7.0	-6.8	-8.4	0.0%	0.0%	0.0%
cyclopropylamine	212-142-2	765-30-0	765300	3716	Reach_1539	3224	4.24	0.93	3				-7.0	-6.8	-8.1	0.0%	0.0%	0.0%
602-964-3	619-529-9	56914-82-0	56914820	3215	Reach_4528	3225	3.85	0.46	3				-7.1	-6.8	-7.9	0.0%	0.0%	0.0%
dicyclohexyl ketone	204-336-0	119-60-8	119608	353	Reach_981	3226	3.47		2				-7.1	-6.8	-8.3	0.0%	0.0%	0.0%
606-080-9	209-800-6	593-60-2	593602	3274	Reach_1395	3227	5.52	0.73	3				-6.6	-6.8	-8.2	0.0%	0.0%	0.0%
605-617-4	605-617-4	17183-98-1	17183981	2124	Reach_4180	3228	3.70	0.69	3				-6.3	-6.8	-8.2	0.0%	0.0%	0.0%
4-Methyl-2,6-bis[(4-methylphenyl)amino]-5-{[2-(trifluoromethyl	601-350-2	115241-16-2	115241162	1634	Reach_4086	3229	6.69	2.34	3				-6.3	-6.8	-8.3	0.0%	0.0%	0.0%
oxalyl dichloride	225-791-1	5080-22-8	5080228	3019	Reach_2076	3230	4.85	1.10	3	4.08	1.20		-7.2	-6.8	-8.7	0.0%	0.0%	0.0%
614-050-1	606-524-1	203313-47-7	203313477	2260	Reach_4210	3231	3.50	0.75	3				-6.6	-6.8	-7.9	0.0%	0.0%	0.0%
propyltriacetoxysilane	241-816-9	17865-07-5	17865075	2155	Reach_2446	3232	5.71	0.90	3	4.66	0.52		-7.0	-6.9	-8.4	0.0%	0.0%	0.0%
2,2,2-trichloro-1-phenylethyl acetate	201-972-0	90-17-5	90175	3992	Reach_360	3233	4.38	0.19	3	3.38	0.19		-7.1	-6.9	-8.2	0.0%	0.0%	0.0%
2-tert-butylaminoethyl methacrylate	223-228-4	3775-90-4	3775904	2806	Reach_1990	3234	4.73		1				-7.1	-6.9	-8.4	0.0%	0.0%	0.0%
pent-3-enenitrile	805-364-1	1170722-65-2	1170722652	5614	Reach_5064	3235							-7.1	-6.9	-7.9	0.0%	0.0%	0.0%
diethyl sulphide	206-526-9	352-93-2	352932	2728	Reach_1244	3236	4.66		2				-7.1	-6.9	-8.7	0.0%	0.0%	0.0%
(2Z)-3-(3-chloro-2-fluorophenyl)-2-(4-chloro-2-fluorophenyl)acry	692-614-6	5660-53-7	5660537	3205	Reach_4677	3237	5.56		1				-7.0	-6.9	-7.7	0.0%	0.0%	0.0%
(vinyloxy)cyclohexane	210-484-7	616-47-7	616477	3346	Reach_1433	3238	5.28	0.13	3	4.42	0.18		-7.1	-6.9	-8.4	0.0%	0.0%	0.0%
dimethyl octadecylphosphonate	246-904-0	25371-54-4	25371544	2432	Reach_2567	3239	1.44	0.81	3				-6.8	-6.9	-8.0	0.0%	0.0%	0.0%
dimethoxymethylsilane	240-914-9	16881-77-9	16881779	2115	Reach_2429	3240	7.27	0.86	3	5.42	1.07		-7.1	-6.9	-8.4	0.0%	0.0%	0.0%
614-707-2	614-707-2	68684-63-9	68684639	3524	Reach_4400	3241	2.19	0.35	3				-6.6	-6.9	-8.0	0.0%	0.0%	0.0%
ethyl 5-oxo-1-phenyl-2-pyrazoline-3-carboxylate	275-177-2	71077-34-4	71077344	6008	Reach_2926	3242							-6.1	-6.9	-8.4	0.0%	0.0%	0.0%
N-methylisopropylamine	225-266-7	4747-21-1	4747211	2967	Reach_2061	3243	4.69	0.44	3	3.69	0.44		-7.1	-6.9	-8.2	0.0%	0.0%	0.0%
cineole	207-431-5	470-82-6	470826	645	Reach_1287	3244	4.97	0.70	20	4.19	0.70		-7.1	-6.9	-9.0	0.0%	0.0%	0.0%
p-tert-butylstyrene	217-126-9	1746-23-2	1746232	2139	Reach_1716	3245	3.39	0.21	3	2.39	0.21		-7.1	-6.9	-8.8	0.0%	0.0%	0.0%
1,1,3,3-tetramethylbutyl hydroperoxide	227-369-2	5809-08-5	5809085	1277	Reach_2136	3246	3.79		2				-7.1	-6.9	-8.1	0.0%	0.0%	0.0%
butyl hydrogen maleate	213-116-3	925-21-3	925213	4038	Reach_1596	3247	4.49	0.37	3	3.79	0.52		-6.3	-6.9	-8.5	0.0%	0.0%	0.0%
ethyl methyl sulphide	210-868-4	624-89-5	624895	3373	Reach_1455	3248	4.85		2				-7.1	-6.9	-8.6	0.0%	0.0%	0.0%
1-[4-({4-[(E)-{5-acetamido-2-methoxy-4-[(E)-(3,6,8-trisulfo-2-nap	700-803-2	14531-84-1	14531841	1984	Reach_4998	3249	4.30		1				-6.6	-6.9	-8.2	0.0%	0.0%	0.0%
1-[4-amino-6-({4-[(E)-(4,8-disulfo-2-naphthyl)diazenyl]-8-sulfo-1-	215-947-7	1458-18-0	1458180	1989	Reach_1684	3250	2.66		2				-6.6	-6.9	-8.2	0.0%	0.0%	0.0%
3,4-dichlorobut-1-ene	617-707-0	85390-93-8	85390938	3885	Reach_4471	3251	3.95	0.94	3				-7.1	-6.9	-8.5	0.0%	0.0%	0.0%
sodium 2-amino-5-nitrobenzenesulphonate	691-442-9	1316184-44-7	1316184447	5661	Reach_4668	3252							-6.6	-6.9	-8.2	0.0%	0.0%	0.0%
2-[(o-nitrophenyl)azo]-p-cresol	615-275-8	71301-98-9	71301989	3579	Reach_4413	3253	4.47		1				-6.5	-6.9	-8.3	0.0%	0.0%	0.0%
1-bromobutane	203-691-9	109-65-9	109659	259	Reach_782	3254	4.56		1				-7.1	-6.9	-8.9	0.0%	0.0%	0.0%
1-cyanocyclopropanaminium chloride	700-563-9	72621-59-1	72621591	3608	Reach_4936	3255	4.25	0.72	3				-6.6	-6.9	-8.2	0.0%	0.0%	0.0%
2-Fluoro-5-(methylsulfonyl)benzoic acid	689-137-0	247569-56-8	247569568	2403	Reach_4647	3256	4.97	0.61	3				-6.0	-6.9	-8.6	0.0%	0.0%	0.0%
1-methyltrimethylene dimethacrylate	213-650-7	998-30-1	998301	4219	Reach_1630	3257	3.67	0.66	3				-7.1	-6.9	-8.3	0.0%	0.0%	0.0%
α,α,2,6-tetrachlorotoluene	221-660-8	3179-76-8	3179768	2637	Reach_1929	3258	5.58	0.96	3	4.58	0.96		-7.1	-6.9	-8.2	0.0%	0.0%	0.0%
1,1,4,4-tetramethylbutane-1,4-diyl bis(2-ethylperoxyhexanoate)	235-935-5	13052-09-0	13052090	1839	Reach_2322	3259	5.00		1				-6.8	-6.9	-8.2	0.0%	0.0%	0.0%
isopropyl acetoacetate	208-798-4	542-08-5	542085	3135	Reach_1345	3260	4.60	1.03	3				-7.1	-6.9	-8.4	0.0%	0.0%	0.0%
anthracene-9-carbaldehyde	678-409-4	18402-22-7	18402227	2189	Reach_4618	3261	2.65	0.73	3				-6.9	-6.9	-8.4	0.0%	0.0%	0.0%
4'-hydroxyacetophenone	202-802-8	99-93-4	99934	4222	Reach_542	3262	4.32	0.43	3	3.41	0.41		-6.7	-6.9	-8.5	0.0%	0.0%	0.0%
(Z)-1,3-dichloropropene	233-195-8	10061-01-5	10061015	132	Reach_2279	3263	3.43	0.66	6	2.41	0.70		-7.2	-6.9	-8.5	0.0%	0.0%	0.0%

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Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
benzenethiol	203-321-6	105-67-9	105679	181	Reach_647	3264	3.80	0.84	32	2.80	0.84		-7.1	-6.9	-8.0	0.0%	0.0%	0.0%
3a,4,5,6,7,7a-hexahydro-4,7-methanoinden-6-yl acetate	226-501-6	5413-60-5	5413605	3128	Reach_2106	3265	4.25	0.20	3	3.25	0.20		-7.1	-6.9	-8.4	0.0%	0.0%	0.0%
800-188-1	800-188-1	33626-25-4	33626254	2683	Reach_5039	3266	3.57	0.23	3				-7.2	-6.9	-9.2	0.0%	0.0%	0.0%
diethyl 4,4'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[4,5	200-983-8	76-74-4	76744	876	Reach_176	3267	4.69		1				-6.8	-6.9	-7.4	0.0%	0.0%	0.0%
iodomethane	233-892-7	10416-59-8	10416598	1386	Reach_2291	3268							-7.3	-6.9	-9.0	0.0%	0.0%	0.0%
3-methoxyestra-2,5(10)-dien-17β-ol	214-130-2	1091-93-6	1091936	1496	Reach_1645	3269	1.69		2				-6.4	-6.9	-8.3	0.0%	0.0%	0.0%
2,3,4-trichlorobut-1-ene	617-344-8	82543-09-7	82543097	3826	Reach_4452	3270	2.48		1				-7.2	-6.9	-8.4	0.0%	0.0%	0.0%
(ethoxymethoxy)cyclododecane	261-332-1	58567-11-6	58567116	3249	Reach_2830	3271	3.74	0.86	3	2.94	0.56		-7.1	-6.9	-8.2	0.0%	0.0%	0.0%
difluoroacetic acid	206-839-0	381-73-7	381737	2818	Reach_1262	3272	6.49	1.24	3	5.49	1.24		-6.0	-6.9	-8.6	0.0%	0.0%	0.0%
dichlorocyclohexylmethylsilane	226-956-0	5578-42-7	5578427	3177	Reach_2125	3273	4.49	0.36	3	3.41	0.30		-7.2	-6.9	-9.2	0.0%	0.0%	0.0%
608-307-7	619-021-7	94361-26-9	94361269	4104	Reach_4508	3274	2.11		1				-7.1	-6.9	-8.1	0.0%	0.0%	0.0%
4-tert-butyl-2-(5-tert-butyl-2-oxo-2,3-dihydro-1-benzofuran-3-yl	700-641-2	1261240-30-5	1261240305	1802	Reach_4957	3275	-0.61	0.88	3				-7.0	-6.9	-7.4	0.0%	0.0%	0.0%
(2-chloro-5-iodophenyl)(4-fluorophenyl)methanone	619-596-4	915095-86-2	915095862	4017	Reach_4532	3276	2.87	0.11	3				-7.1	-6.9	-7.9	0.0%	0.0%	0.0%
trimethoxyoctylsilane	221-338-7	3069-40-7	3069407	2609	Reach_1910	3277	3.37	1.66	3	2.37	1.66		-7.1	-6.9	-8.2	0.0%	0.0%	0.0%
2-[(E)-(4-{[4-(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)butyl](ethyl)	700-154-5	1034138-69-6	1034138696	1365	Reach_4782	3278	2.57	1.11	3				-6.6	-6.9	-8.4	0.0%	0.0%	0.0%
611-025-7	611-025-7	53651-69-7	53651697	3107	Reach_4346	3279	5.81	0.51	3	4.81	0.51		-7.1	-6.9	-8.5	0.0%	0.0%	0.0%
ethyl trifluoroacetate	206-851-6	383-63-1	383631	621	Reach_1263	3280	6.12	1.46	3	5.12	1.46		-7.2	-6.9	-8.5	0.0%	0.0%	0.0%
800-278-0	800-278-0	41435-93-2	41435932	2876	Reach_5040	3281	4.54	0.17	3				-7.2	-6.9	-8.5	0.0%	0.0%	0.0%
2-chloro-3-oxopentyl acetate	695-685-1	1360540-27-7	1360540277	5675	Reach_4693	3282							-7.1	-6.9	-8.4	0.0%	0.0%	0.0%
triethoxypropylsilane	219-842-7	2550-02-9	2550029	1250	Reach_1836	3283	5.73	0.84	3	4.73	0.84		-7.2	-6.9	-8.2	0.0%	0.0%	0.0%
m-bis(1-methylvinyl)benzene	223-146-9	3748-13-8	3748138	2798	Reach_1988	3284	3.70	0.10	3	2.70			-7.2	-6.9	-8.6	0.0%	0.0%	0.0%
3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl methacrylate	218-407-9	2144-53-8	2144538	2294	Reach_1763	3285	2.57	0.43	3	3.49			-7.1	-6.9	-9.6	0.0%	0.0%	0.0%
bisisobutyryl peroxide	222-340-0	3437-84-1	3437841	2701	Reach_1961	3286	5.33	0.33	3	4.33	0.33		-7.2	-6.9	-8.4	0.0%	0.0%	0.0%
2-ethylhexyl benzoate	226-641-8	5444-75-7	5444757	3144	Reach_2113	3287	3.91		1				-7.1	-6.9	-8.2	0.0%	0.0%	0.0%
619-021-7	216-832-4	1678-25-7	1678257	2112	Reach_1707	3288	3.60	0.87	3				-7.1	-6.9	-8.1	0.0%	0.0%	0.0%
p-mentha-1,4(8)-diene	209-578-0	586-62-9	586629	731	Reach_1386	3289	3.37	0.70	7	2.37	0.70		-7.2	-6.9	-9.0	0.0%	0.0%	0.0%
theophyllin-7-ylacetic acid	700-009-6	144333-84-6	144333846	1975	Reach_4724	3290	5.38	2.13	3				-5.9	-6.9	-8.7	0.0%	0.0%	0.0%
2-methoxy-5-(2-oxopropyl)benzenesulfonamide	611-489-0	57260-71-6	57260716	3227	Reach_4360	3291	4.28	0.87	3				-6.1	-6.9	-8.7	0.0%	0.0%	0.0%
methylphosphonous dichloride	700-007-5	95709-83-4	95709834	4130	Reach_4722	3292	2.99	0.12	3				-7.3	-6.9	-8.9	0.0%	0.0%	0.0%
Tris{4-[(4-acetylphenyl)sulfanyl]phenyl}sulfonium hexafluorophc	700-373-6	953084-13-4	953084134	6092	Reach_4878	3293							-6.7	-6.9	-8.3	0.0%	0.0%	0.0%
[1R-(1α,2β,4β,6α)]-2,2,7-trimethyl-3-oxatricyclo[4.1.1.02,4]octar	208-704-1	538-75-0	538750	3114	Reach_1334	3294	3.29	0.06	3				-7.2	-7.0	-8.3	0.0%	0.0%	0.0%
barium bis[5-chloro-4-ethyl-2-[(2-hydroxy-1-naphthyl)azo]benze	267-122-6	67801-01-8	67801018	5987	Reach_2888	3295	4.97	1.01	3	3.97	1.01		-6.7	-7.0	-8.3	0.0%	0.0%	0.0%
1-(dichloromethyl)-2-(trichloromethyl)benzene	246-928-1	25383-06-6	25383066	2433	Reach_2568	3296	5.68	1.29	3				-7.2	-7.0	-8.1	0.0%	0.0%	0.0%
2-ethoxy-4,6-difluoropyrimidine	230-049-5	6925-69-5	6925695	3537	Reach_2212	3297	5.18	0.14	3	3.93	0.47		-7.2	-7.0	-8.1	0.0%	0.0%	0.0%
3,7-dimethyloctan-1-ol	203-374-5	106-21-8	106218	1431	Reach_658	3298	4.08	0.45	3	3.08	0.45		-7.2	-7.0	-8.2	0.0%	0.0%	0.0%
1,3-butylene diacetate	201-200-2	79-37-8	79378	3773	Reach_242	3299	5.06	0.63	3				-7.1	-7.0	-8.3	0.0%	0.0%	0.0%
fluoroethylene	277-620-5	73833-37-1	73833371	6018	Reach_2941	3300							-7.3	-7.0	-8.8	0.0%	0.0%	0.0%
diethyl ethoxymethylenemalonate	201-725-7	87-13-8	87138	3919	Reach_307	3301	3.80	0.77	3				-7.1	-7.0	-8.5	0.0%	0.0%	0.0%
(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl (2R,5R)-5-hydroxy-1,3	604-569-1	147126-62-3	147126623	1996	Reach_4158	3302	4.89		2				-6.3	-7.0	-8.5	0.0%	0.0%	0.0%
tetrasodium 4,4'-bis[[4-[(2-hydroxyethyl)amino]-6-(m-sulphonat	240-400-4	16324-27-9	16324279	5731	Reach_2418	3303				4.16			-6.7	-7.0	-8.3	0.0%	0.0%	0.0%
tripotassium hydrogen ethylenediaminetetraacetate	700-414-8	23328-71-4	23328714	5784	Reach_4892	3304	1.51	0.34	3	0.61	0.43		-6.7	-7.0	-8.3	0.0%	0.0%	0.0%
N,N,N-Trimethyl-3-(octadecyloxy)propan-1-ammonium chloride	611-909-2	59875-04-6	59875046	3292	Reach_4367	3305	4.60	1.39	3				-6.7	-7.0	-8.3	0.0%	0.0%	0.0%
ethyl 4-hydroxy-2-methyl-2H-1,2-benzothiazine-3-carboxylate 1,	604-604-0	147770-06-7	147770067	1998	Reach_4159	3306	1.96	0.16	3				-6.1	-7.0	-8.7	0.0%	0.0%	0.0%
4,6-Dinitro-2,1,3-benzoxadiazole 1-oxide	207-101-0	434-22-0	434220	2913	Reach_1274	3307	4.11	0.58	3				-6.2	-7.0	-8.7	0.0%	0.0%	0.0%
3-p-cumenyl-2-methylpropionaldehyde	203-161-7	103-95-7	103957	1382	Reach_617	3308	3.41	0.20	3	2.41	0.20		-7.2	-7.0	-9.3	0.0%	0.0%	0.0%
1,4-diethylbenzene	203-265-2	105-05-5	105055	1405	Reach_635	3309	3.62	0.44	3	2.62	0.44		-7.2	-7.0	-8.8	0.0%	0.0%	0.0%
3,4-dihydro-2H-pyran	201-487-4	83-56-7	83567	3849	Reach_283	3310	3.50	0.34	3				-7.2	-7.0	-8.6	0.0%	0.0%	0.0%
nitroethane	201-188-9	79-24-3	79243	3769	Reach_237	3311	5.31	1.02	3	4.31	1.00		-7.2	-7.0	-8.3	0.0%	0.0%	0.0%
trimethoxy(2-methylpropyl)silane	250-437-8	31024-56-3	31024563	2617	Reach_2650	3312	5.08	0.55	3	4.08	0.55		-7.2	-7.0	-8.4	0.0%	0.0%	0.0%
triethoxysilane	214-711-0	1189-08-8	1189088	1682	Reach_1669	3313	4.51	0.52	3	3.51	0.52		-7.2	-7.0	-8.3	0.0%	0.0%	0.0%
benzyl chloroformate	240-596-1	16529-56-9	16529569	2098	Reach_2423	3314	4.89		1				-7.2	-7.0	-8.6	0.0%	0.0%	0.0%
diethyl N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]be	222-158-1	3373-59-9	3373599	2685	Reach_1953	3315	5.45	1.21	3				-6.1	-7.0	-8.7	0.0%	0.0%	0.0%
Potassium di-tert-butyl phosphate	240-387-5	16298-03-6	16298036	2087	Reach_2417	3316	4.85		1				-6.7	-7.0	-8.3	0.0%	0.0%	0.0%
1,1'-(1,3-dioxolane-2,2-diyldimethanediyl)bis(1H-1,2,4-triazole)	254-154-0	38849-09-1	38849091	2826	Reach_2719	3317	2.87	0.52	3				-6.1	-7.0	-8.7	0.0%	0.0%	0.0%
2,4-Di-tert-butyl-5-nitrophenyl methyl carbonate	695-104-1	52980-28-6	52980286	3083	Reach_4687	3318							-7.1	-7.0	-8.3	0.0%	0.0%	0.0%
bromotrimethylsilane	224-481-3	4378-61-4	4378614	2916	Reach_2030	3319	3.67	0.29	3	2.67	0.29		-7.5	-7.0	-9.2	0.0%	0.0%	0.0%
4-chloro-1-(dichloromethyl)benzene	296-417-2	92671-67-5	92671675	4043	Reach_2996	3320	5.18		1				-7.2	-7.0	-8.5	0.0%	0.0%	0.0%
tetrapropyl orthosilicate	209-790-3	593-45-3	593453	3273	Reach_1393	3321	7.67		1				-7.2	-7.0	-8.7	0.0%	0.0%	0.0%
diethyl dipropylmalonate	220-928-1	2941-64-2	2941642	2565	Reach_1889	3322	3.89	1.08	3				-7.2	-7.0	-8.5	0.0%	0.0%	0.0%
thioacetic acid	208-063-8	507-09-5	507095	3016	Reach_1315	3323	3.53		1				-6.2	-7.0	-8.6	0.0%	0.0%	0.0%
veratric acid	617-252-8	81653-77-2	81653772	3810	Reach_4449	3324	4.92		1				-6.4	-7.0	-8.6	0.0%	0.0%	0.0%
1-(3-tert-butyl-5-iodo-4-methoxyphenyl)pyrimidine-2,4(1H,3H)-c	800-476-7	1132940-53-4	1132940534	1617	Reach_5046	3325	3.14	0.55	3				-6.5	-7.0	-8.4	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
691-865-9	691-865-9	17696-64-9	17696649	2149	Reach_4672	3326	4.18	1.49	3				-7.2	-7.0	-8.2	0.0%	0.0%	0.0%
sodium 3-((2,3-dicyanophenyl)sulfonyl)propane-1-sulfonate	696-126-4	886592-17-2	886592172	6076	Reach_4706	3327							-6.7	-7.0	-8.4	0.0%	0.0%	0.0%
1,3-dichlorobut-2-ene	606-738-5	213265-81-7	213265817	2289	Reach_4215	3328	3.44		2				-7.3	-7.0	-8.6	0.0%	0.0%	0.0%
2,6,8-trimethylnonan-4-ol	229-554-3	6607-34-7	6607347	3461	Reach_2196	3329	4.29	0.84	3				-7.2	-7.0	-8.4	0.0%	0.0%	0.0%
nonane	225-083-2	4651-67-6	4651676	2954	Reach_2053	3330	5.37	0.22	3	4.37	0.22		-7.3	-7.0	-9.3	0.0%	0.0%	0.0%
N,N'-(2,5-dimethyl-1,4-phenylene)bis[4-[(5-chloro-2-methylphen	279-211-7	79665-24-0	79665240	3779	Reach_2956	3331	-0.97	3.47	3	4.00			-7.2	-7.0	-6.0	0.0%	0.0%	0.0%
609-534-4	609-534-4	382-26-3	382263	2819	Reach_4305	3332							-7.3	-7.0	-9.5	0.0%	0.0%	0.0%
2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-meth	200-396-7	58-73-1	58731	3253	Reach_48	3333	3.16	0.50	3				-6.7	-7.0	-8.5	0.0%	0.0%	0.0%
4-{2-[2-(2-Chloro-3-{2-[1,1-dimethyl-3-(4-sulfobutyl)-1H-benzo[e	700-626-0	1073607-50-7	1073607507	5603	Reach_4954	3334							-6.7	-7.0	-8.4	0.0%	0.0%	0.0%
5-[[(2-aminoethyl)thio]methyl]-N,N-dimethyl-2-furfurylamine	616-285-5	76028-96-1	76028961	3694	Reach_4430	3335	4.63	0.41	3				-6.3	-7.0	-8.7	0.0%	0.0%	0.0%
tetrahydro-3-methylfuran	236-537-4	13423-15-9	13423159	1876	Reach_2335	3336	6.86	0.44	3	5.86	0.44		-7.2	-7.0	-8.3	0.0%	0.0%	0.0%
O,O-diisobutyl hydrogen dithiophosphate	252-549-2	35410-28-7	35410287	2731	Reach_2689	3337	4.78	0.93	3				-7.2	-7.0	-8.2	0.0%	0.0%	0.0%
pentadecane	211-098-1	629-62-9	629629	772	Reach_1469	3338	5.67	1.43	4	4.67	0.70		-7.0	-7.0	-8.8	0.0%	0.0%	0.0%
5-ethyl-5-(1-methylbutyl)-2-thiobarbituric acid	700-683-1	853950-77-3	853950773	3887	Reach_4966	3339	4.24	0.85	3				-6.5	-7.0	-8.4	0.0%	0.0%	0.0%
607-988-8	610-651-8	51336-95-9	51336959	3035	Reach_4333	3340	2.25	0.51	3				-6.5	-7.0	-8.5	0.0%	0.0%	0.0%
8,9-Difluoro-3-methyl-6-oxo-2,3-dihydro-6H-1-oxa-3a-aza-phena	607-317-9	24085-06-1	24085061	2372	Reach_4237	3341	3.08	0.36	3	2.08	0.36		-6.3	-7.0	-8.7	0.0%	0.0%	0.0%
2,3-epoxybutane	276-173-3	71902-23-3	71902233	3594	Reach_2933	3342	4.96	0.97	3	4.49	0.95		-7.2	-7.0	-8.4	0.0%	0.0%	0.0%
6-methylhept-5-en-2-one	272-574-2	68890-66-4	68890664	5998	Reach_2911	3343	3.39	0.45	3	2.77	0.36		-7.2	-7.0	-8.2	0.0%	0.0%	0.0%
4'-ethoxy-3-hydroxy-2-naphthanilide	212-157-4	766-05-2	766052	873	Reach_1541	3344	4.74	0.46	3				-6.5	-7.0	-8.3	0.0%	0.0%	0.0%
di-tert-pentyl peroxide	234-042-8	10508-09-5	10508095	1406	Reach_2293	3345	4.37		1				-7.3	-7.0	-9.2	0.0%	0.0%	0.0%
ethyl (3S)-9,10-difluoro-3-methyl-7-oxo-2,3-dihydro-7H-[1,4]oxa	242-500-3	18683-91-5	18683915	2204	Reach_2467	3346	3.61	0.64	3				-6.2	-7.0	-8.7	0.0%	0.0%	0.0%
619-072-5	224-262-2	4271-96-9	4271969	2897	Reach_2024	3347	4.80	1.07	3				-6.6	-7.0	-8.7	0.0%	0.0%	0.0%
5-bromo-1H-pyrrolo[2,3-b]pyridine	700-129-9	2004-62-8	2004628	2249	Reach_4772	3348	4.69		2				-6.4	-7.0	-8.6	0.0%	0.0%	0.0%
4-[[4-(aminocarbonyl)phenyl]azo]-3-hydroxy-N-(2-methoxyphen	804-749-1	1216942-02-7	1216942027	1733	Reach_5058	3349	3.24	0.29	3				-6.8	-7.0	-8.6	0.0%	0.0%	0.0%
N-[2-[4-(aminosulphonyl)phenyl]ethyl]-5-chloro-2-methoxybenz	700-141-4	117570-53-3	117570533	1659	Reach_4778	3350	3.65	0.38	3				-6.4	-7.0	-8.7	0.0%	0.0%	0.0%
4-[[5-[[[4-(aminocarbonyl)phenyl]amino]carbonyl]-2-methoxyph	261-785-5	59487-23-9	59487239	3279	Reach_2837	3351	5.04	1.10	3	4.04	1.10		-6.8	-7.0	-8.0	0.0%	0.0%	0.0%
2-Methoxy-4-(trifluoromethyl)pyridine	619-682-1	224049-04-1	224049041	2333	Reach_4535	3352	3.33	0.25	3	2.33	0.25		-7.3	-7.0	-8.4	0.0%	0.0%	0.0%
isopentyl laurate	228-626-1	6309-51-9	6309519	3394	Reach_2164	3353	6.00	1.18	3	5.00	1.18		-7.1	-7.0	-8.6	0.0%	0.0%	0.0%
Benzyl {5-[N-acetyl(hydroxy)amino]pentyl}carbamate	700-416-9	92700-68-0	92700680	4044	Reach_4893	3354	4.10	0.75	3				-6.2	-7.0	-8.6	0.0%	0.0%	0.0%
dodecyloxirane	221-781-6	3234-28-4	3234284	2647	Reach_1935	3355	2.29	0.38	3				-7.3	-7.0	-9.3	0.0%	0.0%	0.0%
619-402-8	619-402-8	99189-60-3	99189603	4198	Reach_4517	3356	5.17	0.52	3	4.17	0.52		-6.3	-7.0	-8.6	0.0%	0.0%	0.0%
chlorocyclopentane	200-740-6	70-54-2	70542	3565	Reach_97	3357	4.28	1.01	3				-7.3	-7.0	-9.0	0.0%	0.0%	0.0%
2-ethylhex-2-enal	213-138-3	926-57-8	926578	4041	Reach_1597	3358	2.51		1				-7.3	-7.0	-8.2	0.0%	0.0%	0.0%
2-ethylhexenal	266-097-9	66063-15-8	66063158	3459	Reach_2875	3359	3.86	0.72	3	2.33	1.61		-7.3	-7.0	-8.2	0.0%	0.0%	0.0%
3,3'-(hexane-1,6-diyldiimino)dipropanenitrile	700-374-1	70918-00-2	70918002	3575	Reach_4879	3360	4.60	1.20	3				-6.3	-7.0	-8.6	0.0%	0.0%	0.0%
tetradecyloxirane	203-783-9	110-61-2	110612	1525	Reach_820	3361	1.40		1				-7.2	-7.0	-9.3	0.0%	0.0%	0.0%
5-[4'-(Bromomethyl)biphenyl-2-yl]-1-trityl-1H-tetrazole	250-185-9	30414-54-1	30414541	2596	Reach_2646	3362	4.53	1.00	3				-6.9	-7.0	-7.6	0.0%	0.0%	0.0%
3-Chloro-N-hydroxy-2,2-dimethylpropanamide	805-721-1	57625-74-8	57625748	3234	Reach_5070	3363	3.45		2				-6.3	-7.0	-8.6	0.0%	0.0%	0.0%
isopropylcyclohexane	219-641-4	2489-05-6	2489056	5579	Reach_1817	3364	1.57	1.12	4	0.43	0.69		-7.3	-7.0	-9.2	0.0%	0.0%	0.0%
bis[2,2,6,6-tetramethyl-1-(octyloxy)piperidin-4-yl] decanedioate	700-529-3	4224-62-8	4224628	2891	Reach_4923	3365	4.91	0.63	3				-7.2	-7.0	-6.8	0.0%	0.0%	0.0%
Ethyl 4-oxo-1,4-dihydroquinoline-3-carboxylate	604-355-8	143418-49-9	143418499	1966	Reach_4151	3366							-6.3	-7.0	-8.7	0.0%	0.0%	0.0%
N-tert-butylacrylamide	203-505-6	107-58-4	107584	1466	Reach_712	3367	4.93	0.68	3	3.93	0.68		-7.1	-7.0	-8.7	0.0%	0.0%	0.0%
630-348-4	685-497-8	850348-10-6	850348106	6057	Reach_4631	3368							-6.5	-7.0	-8.7	0.0%	0.0%	0.0%
1-(allyloxy)-2-methyl-1-oxopropan-2-yl 2-chloro-5-isocyanatober	695-953-8	204918-22-9	204918229	2267	Reach_4698	3369	3.90	0.56	3	2.90	0.56		-7.2	-7.0	-8.6	0.0%	0.0%	0.0%
(6R,7R)-7-{[(2Z)-2-(2-amino-1,3-thiazol-4-yl)-2-(methoxyimino)ac	616-651-4	787582-75-6	787582756	3756	Reach_4443	3370	1.57	1.04	3				-6.4	-7.1	-8.3	0.0%	0.0%	0.0%
octyl octanoate	218-980-5	2306-88-9	2306889	2344	Reach_1782	3371	5.00		1	5.00			-7.2	-7.1	-8.7	0.0%	0.0%	0.0%
1-(3-(2-methoxy-5-nitrophenoxy)propyl)-4-methylpiperazine	609-748-8	39856-50-3	39856503	2851	Reach_4312	3372	3.13	0.97	3				-6.3	-7.1	-8.7	0.0%	0.0%	0.0%
nonanal	601-329-8	114798-26-4	114798264	1626	Reach_4084	3373	6.20	0.45	3	5.20	0.45		-7.3	-7.1	-8.5	0.0%	0.0%	0.0%
604-275-3	611-210-2	54914-95-3	54914953	5927	Reach_4353	3374	4.92	0.72	3	3.92	0.72		-7.3	-7.1	-8.5	0.0%	0.0%	0.0%
α,α-dichlorotoluene	259-173-8	54464-54-9	54464549	3145	Reach_2799	3375	3.32	0.12	3				-7.3	-7.1	-8.5	0.0%	0.0%	0.0%
2,2-dimethyloxirane	629-664-5	79710-86-4	79710864	3780	Reach_4593	3376	5.15	0.33	3				-7.3	-7.1	-8.6	0.0%	0.0%	0.0%
1-[3-(Hydroxymethyl)pyridin-2-yl)-4-methyl-2-phenylpiperazine	700-560-2	13062-58-3	13062583	1840	Reach_4934	3377	3.03	0.17	3				-6.3	-7.1	-8.7	0.0%	0.0%	0.0%
methyl 3-oxo-3-(thiophen-2-yl)propanoate	224-631-8	4431-83-8	4431838	2921	Reach_2034	3378	6.29	0.87	3	5.29	0.87		-7.2	-7.1	-8.8	0.0%	0.0%	0.0%
4-hydroxy-3,5-dimethoxybenzonitrile	700-251-2	72684-95-8	72684958	3609	Reach_4822	3379	4.46		2				-6.5	-7.1	-8.7	0.0%	0.0%	0.0%
2-[methyl[(nonafluorobutyl)sulphonyl]amino]ethyl acrylate	266-733-5	67584-55-8	67584558	3497	Reach_2886	3380	3.08		1				-7.3	-7.1	-8.5	0.0%	0.0%	0.0%
barium bis[2-[(2-hydroxynaphthyl)azo]naphthalenesulphonate]	214-160-6	1103-38-4	1103384	5606	Reach_1646	3381	4.97	1.01	3	3.97	1.01		-6.8	-7.1	-8.4	0.0%	0.0%	0.0%
(1R)-2-{[2-(4-aminophenyl)ethyl]amino}-1-phenylethanol hydroc	611-111-4	54197-66-9	54197669	3132	Reach_4349	3382	3.71	0.54	3				-6.2	-7.1	-8.7	0.0%	0.0%	0.0%
2-[4-(Dibenzo[b,f][1,4]thiazepin-11-yl)piperazin-1-yl] ethanol	600-417-3	103312-62-5	103312625	1363	Reach_4063	3383	3.26	1.13	3				-6.4	-7.1	-8.7	0.0%	0.0%	0.0%
2-chloro-2-methylpropane	213-212-5	930-28-9	930289	4056	Reach_1605	3384	4.64	0.29	3				-7.3	-7.1	-9.3	0.0%	0.0%	0.0%
trifluoro(trifluoromethyl)oxirane	207-050-4	428-59-1	428591	2900	Reach_1270	3385	3.96		1				-7.3	-7.1	-9.4	0.0%	0.0%	0.0%
1,4-diisopropylbenzene	202-826-9	100-18-5	100185	1296	Reach_550	3386	2.92	0.37	3	2.23	0.26		-7.3	-7.1	-9.3	0.0%	0.0%	0.0%
ethyl 2-methylbutyrate	231-225-4	7452-79-1	7452791	3639	Reach_2252	3387	4.06	0.85	3	3.34			-7.3	-7.1	-8.7	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
607-317-9	200-517-3	61-76-7	61767	5952	Reach_60	3388	3.58		1				-7.1	-7.1	-8.7	0.0%	0.0%	0.0%
1,1,1,3,3,3-hexafluoropropan-2-ol	228-705-0	6330-25-2	6330252	3398	Reach_2165	3389	4.56	1.35	3				-7.3	-7.1	-9.0	0.0%	0.0%	0.0%
2-chloro-N-cyclohexyl-N-(cyclohexylcarbamoyl) acetamide	202-479-3	96-12-8	96128	1045	Reach_451	3390	4.51	0.80	15	3.51	0.80		-6.6	-7.1	-8.7	0.0%	0.0%	0.0%
2,3-dichloropropene	696-185-6	1407097-19-1	1407097191	5683	Reach_4137	3391							-7.4	-7.1	-8.9	0.0%	0.0%	0.0%
1-[1,6-dimethyl-3-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]ethai	700-585-9	35786-94-8	35786948	2749	Reach_4941	3392	3.51		2				-7.3	-7.1	-8.3	0.0%	0.0%	0.0%
1-isopropyl-4-methylcyclohexane	202-790-4	99-82-1	99821	4218	Reach_539	3393	2.90	0.79	3	1.90	0.79		-7.3	-7.1	-9.4	0.0%	0.0%	0.0%
3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-one	208-796-3	542-02-9	542029	3133	Reach_1343	3394	6.54		1				-7.3	-7.1	-8.7	0.0%	0.0%	0.0%
tetrahydro-4-methylene-2-(2-methyl-1-propenyl)-2H-pyran	700-013-8	95709-82-3	95709823	4129	Reach_4725	3395	3.04	0.37	3				-7.3	-7.1	-8.3	0.0%	0.0%	0.0%
N-[3-(Triethoxysilyl)propyl]formamide	607-654-1	252285-60-2	252285602	2423	Reach_4245	3396	2.05	0.40	3				-6.1	-7.1	-8.7	0.0%	0.0%	0.0%
(1E)-1-(1-Naphthyl)ethanone oxime	613-906-1	66212-25-7	66212257	3467	Reach_4390	3397	4.34	0.19	3				-6.7	-7.1	-8.6	0.0%	0.0%	0.0%
α-[(benzyl-tert-butylamino)methyl]-m-xylene-4,α,α'-triol	246-013-7	24085-03-8	24085038	2371	Reach_2537	3398	3.48	0.33	3				-6.4	-7.1	-8.6	0.0%	0.0%	0.0%
tricyclo[3.3.1.13,7]decane	266-100-3	66068-84-6	66068846	3460	Reach_2876	3399	3.99	0.43	3	2.99	0.43		-7.3	-7.1	-8.6	0.0%	0.0%	0.0%
1-(4-methyl-2-nitrophenylazo)-2-naphthol	219-372-2	2425-85-6	2425856	2382	Reach_1806	3400	2.95	0.91	3				-7.0	-7.1	-8.5	0.0%	0.0%	0.0%
cyclohexyl(ethyl)amine	226-733-8	5459-93-8	5459938	688	Reach_2115	3401	4.57		2				-7.3	-7.1	-8.7	0.0%	0.0%	0.0%
N,N'-hexane-1,6-diylbis[2,2-dimethyl-3-(morpholin-4-yl)propan-1	700-570-7	1217271-49-2	1217271492	1736	Reach_4938	3402	4.81		2				-6.5	-7.1	-8.7	0.0%	0.0%	0.0%
triammonium hydrogen ethylenediaminetetraacetate	240-073-8	15934-01-7	15934017	5727	Reach_2405	3403	4.84	0.78	3	4.51	1.00		-6.8	-7.1	-8.5	0.0%	0.0%	0.0%
4-(4-Nitrophenyl)morpholin-3-one	610-199-1	446292-04-2	446292042	2928	Reach_4325	3404	4.54	1.24	3				-6.3	-7.1	-8.8	0.0%	0.0%	0.0%
2,2-difluoro-benzo[1,3]dioxole-4-carbaldehyde	700-476-6	119895-68-0	119895680	1701	Reach_4908	3405	3.40		2				-7.3	-7.1	-8.5	0.0%	0.0%	0.0%
4-chloro-2,3-dimethylpyridine 1-oxide	700-045-2	104966-97-4	104966974	1404	Reach_4737	3406	2.78	0.19	3				-7.3	-7.1	-8.6	0.0%	0.0%	0.0%
5-aminonaphthalene-2-sulphonic acid	204-351-2	119-79-9	119799	1699	Reach_986	3407	4.16	0.88	3				-6.2	-7.1	-8.9	0.0%	0.0%	0.0%
N-(4-bromobenzyl)-N-pentanoyl-L-valine	601-254-0	113479-65-5	113479655	1621	Reach_4081	3408							-6.7	-7.1	-8.7	0.0%	0.0%	0.0%
allyl hexanoate	223-242-0	3779-63-3	3779633	2809	Reach_1991	3409	5.42	0.52	3	4.42	0.52		-7.3	-7.1	-8.6	0.0%	0.0%	0.0%
dicyclohexylcarbodiimide	243-411-2	19894-99-6	19894996	2245	Reach_2486	3410	4.45	0.22	3				-7.3	-7.1	-9.0	0.0%	0.0%	0.0%
2-phenylethyl cyanoacetate	643-078-7	87855-59-2	87855592	3943	Reach_4612	3411							-7.1	-7.1	-8.7	0.0%	0.0%	0.0%
2-phenoxyaniline	620-225-3	5958-24-7	5958247	3280	Reach_4562	3412							-6.6	-7.1	-8.8	0.0%	0.0%	0.0%
3-cyclohexyl-2-(cyclohexylimino)-1,3-oxazolidin-4-one	700-085-0	329216-67-3	329216673	2670	Reach_4755	3413	3.37	0.31	3				-6.7	-7.1	-8.7	0.0%	0.0%	0.0%
N,N-dimethylbutylamine	213-156-1	927-62-8	927628	1014	Reach_1600	3414	4.48	0.54	4	3.58	0.70		-7.3	-7.1	-8.4	0.0%	0.0%	0.0%
6-amino-4-hydroxynaphthalene-2-sulphonic acid	700-266-4	26184-62-3	26184623	2457	Reach_4830	3415	5.12	0.38	3				-6.2	-7.1	-8.8	0.0%	0.0%	0.0%
[methoxy(dimethyl)silyl]methyl acetate	299-966-6	93918-85-5	93918855	4091	Reach_3003	3416	1.84	0.02	3				-7.3	-7.1	-8.5	0.0%	0.0%	0.0%
1,1,1,2,3-Pentachlorpropane	700-848-8	1247119-33-0	1247119330	5640	Reach_5011	3417							-7.4	-7.1	-8.9	0.0%	0.0%	0.0%
4-amino-2-(trifluoromethyl)benzonitrile	700-293-1	654-70-6	654706	3454	Reach_4847	3418	3.76	0.46	3				-7.3	-7.1	-8.6	0.0%	0.0%	0.0%
Methyl (3aR,7aR)-4-oxooctahydro-1H-indole-1-carboxylate	700-703-9	18667-19-1	18667191	2202	Reach_4973	3419	3.05	0.02	3				-6.3	-7.1	-8.7	0.0%	0.0%	0.0%
3,5-bis{1-[4-(propan-2-yl)phenyl]propan-2-yl}dihydro-1H-[1,3]ox	700-207-2	1001164-15-3	1001164153	1293	Reach_4804	3420	1.28	0.22	3				-6.9	-7.1	-7.9	0.0%	0.0%	0.0%
606-682-1	611-928-6	6001-74-7	6001747	5944	Reach_4369	3421							-6.6	-7.1	-8.7	0.0%	0.0%	0.0%
2,2,5,5-tetramethyl-1,4,2,5-dioxadisilinane	700-669-5	2788-28-5	2788285	5814	Reach_4964	3422							-7.5	-7.1	-9.0	0.0%	0.0%	0.0%
620-465-9	700-259-6	64464-07-9	64464079	5968	Reach_4828	3423							-6.4	-7.1	-8.7	0.0%	0.0%	0.0%
3,5,5-trimethylcyclohex-3-en-1-one	695-943-3	151006-11-0	151006110	5709	Reach_4697	3424							-7.3	-7.1	-8.3	0.0%	0.0%	0.0%
barium bis[6-chloro-4-[(2-hydroxy-1-naphthyl)azo]toluene-3-sul	277-553-1	73612-34-7	73612347	6017	Reach_2940	3425	4.97	1.01	3	3.97	1.01		-6.9	-7.1	-8.5	0.0%	0.0%	0.0%
diisobutyl maleate	238-102-4	14234-82-3	14234823	1954	Reach_2360	3426	3.42	0.26	3				-7.3	-7.1	-8.6	0.0%	0.0%	0.0%
613-906-1	700-765-7	100485-51-6	100485516	1307	Reach_4987	3427	3.27	0.61	3				-6.6	-7.1	-8.7	0.0%	0.0%	0.0%
1-({[(2,5-dioxopyrrolidin-1-yl)oxy]carbonyl}oxy)ethyl 2-methylpr	700-402-2	860035-10-5	860035105	3900	Reach_4888	3428	5.08	1.52	3				-6.2	-7.1	-8.9	0.0%	0.0%	0.0%
3,5-Di(undecan-2-yl)dihydro-1H-[1,3]oxazolo[3,4-c][1,3]oxazole	202-657-0	98-32-8	98328	4182	Reach_504	3429	4.09	0.73	3				-7.2	-7.1	-7.5	0.0%	0.0%	0.0%
3-ethoxypregna-3,5-diene-21,17α-carbolactone	700-664-8	486455-65-6	486455656	2973	Reach_4963	3430	3.10	0.54	3				-6.8	-7.1	-8.5	0.0%	0.0%	0.0%
2-methyl-2,3,4,5,6,7,8,9,10,11,12,13-dodecahydro-1H-cyclopent	606-858-8	21890-09-5	21890095	2310	Reach_4220	3431	2.11	0.39	3				-7.2	-7.1	-9.3	0.0%	0.0%	0.0%
Diethyl pyridine-2,4-dicarboxylate	680-341-5	41438-38-4	41438384	2877	Reach_4625	3432	4.40	0.89	3				-7.3	-7.1	-8.7	0.0%	0.0%	0.0%
chlorocyclohexane	203-113-5	103-45-7	103457	1367	Reach_606	3433	4.29	0.28	3	3.29	0.28		-7.4	-7.1	-8.7	0.0%	0.0%	0.0%
butyl(ethyl)amine	236-415-0	13360-63-9	13360639	1869	Reach_2330	3434	4.21	0.85	3	3.21	0.85		-7.3	-7.1	-8.4	0.0%	0.0%	0.0%
[(1R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methanesulfonic	700-248-6	2766-74-7	2766747	2515	Reach_4820	3435	4.48	0.41	3				-6.9	-7.1	-8.5	0.0%	0.0%	0.0%
tert-butyl {(1S)-2-[(1S,3S,5S)-3-cyano-2-azabicyclo[3.1.0]hex-2-yl	687-691-8	709031-43-6	709031436	3573	Reach_4636	3436	3.90	0.57	3				-6.4	-7.1	-8.6	0.0%	0.0%	0.0%
N,N-dibutylbutan-1-aminium bis[2-(hydroxy-kO)benzoato(2-)-kO	700-536-1	25628-08-4	25628084	5798	Reach_4926	3437	5.53		3	4.53			-6.9	-7.1	-8.5	0.0%	0.0%	0.0%
N,N,N-triethylethanaminium 1,1,2,2,3,3,4,4,4-nonafluorobutane	226-887-6	5534-13-4	5534134	3167	Reach_2122	3438	4.16	0.32	3				-6.9	-7.1	-8.5	0.0%	0.0%	0.0%
2-acetamido-5-chlorobenzenesulfonic acid - pyridine (1:1)	250-882-8	31981-44-9	31981449	2641	Reach_2659	3439	3.91	0.65	3				-6.9	-7.1	-8.5	0.0%	0.0%	0.0%
603-087-9	603-087-9	125700-67-6	125700676	6112	Reach_4111	3440							-6.9	-7.1	-8.5	0.0%	0.0%	0.0%
2,2-dimethoxy-N-{2-oxo-2-[(2-phenylethyl)amino]ethyl}ethanam	700-631-8	102601-34-3	102601343	5592	Reach_4956	3441							-6.9	-7.1	-8.5	0.0%	0.0%	0.0%
690-742-7	700-789-8	14352-61-5	14352615	1967	Reach_4995	3442	4.31		2				-6.9	-7.1	-8.5	0.0%	0.0%	0.0%
sodium 3-(cyclohexylamino)-2-hydroxypropane-1-sulfonate	696-235-7	63432-37-1	63432371	3401	Reach_4710	3443	3.58	0.50	3				-6.9	-7.1	-8.5	0.0%	0.0%	0.0%
L-tryptophan	254-179-7	38888-98-1	38888981	2828	Reach_2720	3444	2.74	0.43	3	2.26	0.83		-6.1	-7.1	-8.8	0.0%	0.0%	0.0%
Lithium naphthalene-2-carboxylate	700-252-8	53595-66-7	53595667	3106	Reach_4823	3445	4.29	1.21	3				-6.9	-7.1	-8.5	0.0%	0.0%	0.0%
6-BROMO-4-PHENYLCHROMAN-2-ONE	610-915-2	52937-90-3	52937903	3082	Reach_4339	3446	3.73	1.11	3				-7.1	-7.1	-8.7	0.0%	0.0%	0.0%
estrone	200-164-5	53-16-7	53167	61	Reach_19	3447	1.11	1.61	5	0.11	1.24		-7.4	-7.1	-8.4	0.0%	0.0%	0.0%
5-Bromo-3-[(1R)-1-(2,6-dichloro-3-fluorophenyl)ethoxy]pyridin-2	689-734-6	39903-01-0	39903010	2852	Reach_4653	3448	3.11	0.94	3				-6.7	-7.1	-8.7	0.0%	0.0%	0.0%
4-amino-N-(2-methylquinolin-8-yl)benzenesulfonamide	604-269-0	14205-46-0	14205460	1945	Reach_4146	3449							-6.6	-7.1	-8.7	0.0%	0.0%	0.0%

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Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
(2Z)-(5-amino-1,2,4-thiadiazol-3-yl){[(1-tert-butoxy-2-methyl-1-o	609-518-7	38089-93-9	38089939	2815	Reach_4303	3450	3.65	0.82	3				-6.6	-7.1	-8.7	0.0%	0.0%	0.0%
methyl benzilate	700-294-7	109010-60-8	109010608	1492	Reach_4848	3451	4.02	1.70	3				-6.5	-7.1	-8.7	0.0%	0.0%	0.0%
3-(dodecylthio)butyronitrile	604-275-3	14214-31-4	14214314	1947	Reach_4147	3452							-7.3	-7.1	-8.4	0.0%	0.0%	0.0%
618-972-5	618-972-5	93771-36-9	93771369	4082	Reach_4505	3453	4.01		1				-6.5	-7.1	-8.6	0.0%	0.0%	0.0%
680-297-7	806-599-2	33125-90-5	33125905	2675	Reach_5077	3454	3.67		2				-6.3	-7.2	-8.7	0.0%	0.0%	0.0%
2-(2-aminopropan-2-yl)-4-[(4-fluorobenzyl)carbamoyl]-1-methyl-	608-783-6	327-78-6	327786	2663	Reach_4283	3455	2.51		1				-6.4	-7.2	-8.7	0.0%	0.0%	0.0%
6-Iodo indazole	620-465-9	2657-85-4	2657854	2479	Reach_4572	3456	4.04	0.77	3				-7.2	-7.2	-8.7	0.0%	0.0%	0.0%
604-355-8	700-139-3	867022-57-9	867022579	3909	Reach_4776	3457	3.00	0.51	3				-6.6	-7.2	-8.7	0.0%	0.0%	0.0%
6-methyl-4-oxo-5,6-dihydro-4H-thieno[2,3-b]thiopyran-2-sulfona	700-296-8	61337-89-1	61337891	3332	Reach_4849	3458	3.85	0.69	3				-6.5	-7.2	-8.7	0.0%	0.0%	0.0%
propane-2-thiol	200-861-4	75-33-2	75332	3667	Reach_139	3459	3.78	0.68	3	2.78	0.68		-7.4	-7.2	-9.1	0.0%	0.0%	0.0%
pentafluoroiodoethane	212-058-6	757-86-8	757868	3688	Reach_1528	3460	2.42	2.18	3				-7.5	-7.2	-9.3	0.0%	0.0%	0.0%
N-[(3R,4R)-1-benzyl-4-methylpiperidin-3-yl]-2-chloro-N-methyl-1	220-513-5	2787-02-2	2787022	1256	Reach_1869	3461	3.55	0.53	3				-6.4	-7.2	-8.7	0.0%	0.0%	0.0%
601-350-2	700-100-0	39716-58-0	39716580	2848	Reach_4762	3462	4.79		2				-6.1	-7.2	-8.7	0.0%	0.0%	0.0%
dibenzo(b,f)cycloheptan-1-one	614-818-6	689293-69-4	689293694	3531	Reach_4401	3463	2.14	0.40	3				-7.4	-7.2	-8.4	0.0%	0.0%	0.0%
3-(1-pyrrolidinyl)propiophenone hydrochloride	212-633-1	833-86-3	833863	6047	Reach_1561	3464							-6.9	-7.2	-8.5	0.0%	0.0%	0.0%
4-(decanoyloxy)benzoic acid	617-941-3	86960-46-5	86960465	3914	Reach_4481	3465	4.41	0.95	3	3.41	0.95		-6.7	-7.2	-8.7	0.0%	0.0%	0.0%
3-phenylbutyraldehyde	240-362-9	16251-77-7	16251777	2085	Reach_2415	3466	4.19		2				-7.4	-7.2	-8.4	0.0%	0.0%	0.0%
N-(5-chloro-2-methoxyphenyl)-3-hydroxy-4-[[2-methoxy-5-[(phe	224-794-5	4498-67-3	4498673	2935	Reach_2041	3467	2.93	2.99	3				-6.8	-7.2	-8.7	0.0%	0.0%	0.0%
tert-butyl piperazine-1-carboxylate	618-533-8	90356-78-8	90356788	3999	Reach_4497	3468	3.03	0.50	3				-7.3	-7.2	-8.7	0.0%	0.0%	0.0%
dichloromethyl(3,3,3-trifluoropropyl)silane	211-623-4	675-62-7	675627	3496	Reach_1495	3469	4.64	0.42	3	3.64	0.42		-7.5	-7.2	-9.4	0.0%	0.0%	0.0%
4-[2-(benzylamino)propyl]phenol	225-511-8	4890-85-1	4890851	2979	Reach_2066	3470	3.11		1				-6.5	-7.2	-8.7	0.0%	0.0%	0.0%
615-027-9	615-027-9	69904-10-5	69904105	3552	Reach_4406	3471	4.43		2				-6.2	-7.2	-8.9	0.0%	0.0%	0.0%
4'-chloro-3-hydroxy-2-naphthanilide	204-248-2	118-41-2	118412	1668	Reach_962	3472	4.66	0.43	3				-6.6	-7.2	-8.5	0.0%	0.0%	0.0%
3-chlorophthalic anhydride	620-285-0	902146-43-4	902146434	3994	Reach_4563	3473	4.24	1.15	3				-7.4	-7.2	-8.5	0.0%	0.0%	0.0%
608-291-1	211-814-2	698-29-3	698293	3550	Reach_1513	3474	5.91		1				-7.4	-7.2	-8.9	0.0%	0.0%	0.0%
1,1'-(1,3-Phenylenedicarbonyl)diazepan-2-one	700-226-6	488097-90-1	488097901	2976	Reach_4811	3475	4.10	0.81	3				-6.4	-7.2	-8.7	0.0%	0.0%	0.0%
ethyl 1-(4-methoxyphenyl)-7-oxo-6-[4-(2-oxopiperidin-1-yl)phen	253-292-9	36968-27-1	36968271	2786	Reach_2708	3476	2.81	0.95	3	4.48			-6.8	-7.2	-8.7	0.0%	0.0%	0.0%
oleoyl chloride	616-210-6	75302-98-6	75302986	3665	Reach_4427	3477	2.39	0.74	3				-7.3	-7.2	-9.0	0.0%	0.0%	0.0%
2,6,6-trimethylbicyclo[3.1.1]heptane-3-carbaldehyde	619-372-6	98730-04-2	98730042	4191	Reach_4515	3478	3.83	0.45	3	2.79	0.43		-7.4	-7.2	-8.4	0.0%	0.0%	0.0%
610-150-4	700-627-6	17270-01-8	17270018	2130	Reach_4955	3479	5.50		3	4.50			-6.9	-7.2	-8.5	0.0%	0.0%	0.0%
639-259-5	639-259-5	104366-82-7	104366827	1391	Reach_4603	3480	3.47	0.52	3				-6.2	-7.2	-8.8	0.0%	0.0%	0.0%
N-(dimethylvinylsilyl)-1,1-dimethyl-1-vinylsilylamine	231-701-1	7691-02-3	7691023	1290	Reach_2269	3481	5.30	0.46	3	4.19	0.63		-7.4	-7.2	-9.3	0.0%	0.0%	0.0%
Nonylphenol, ethoxylated	500-024-6	9016-45-9	9016459	1001	Reach_4050	3482	3.87	0.68	21	2.87	0.68	21	-6.6	-7.2	-8.4	0.0%	0.0%	0.0%
N-ethylmethacrylamine	242-217-5	18328-90-0	18328900	2182	Reach_2459	3483							-7.4	-7.2	-8.6	0.0%	0.0%	0.0%
4,4'-methylenebis(N-sec-butylcyclohexanamine)	217-101-2	1739-84-0	1739840	2135	Reach_1715	3484	4.88	0.31	3	3.88	0.31		-7.3	-7.2	-8.7	0.0%	0.0%	0.0%
tert-butyl peroxyisobutyrate	239-032-7	14960-06-6	14960066	5705	Reach_2374	3485	3.87	0.53	3	2.87	0.53		-7.4	-7.2	-8.8	0.0%	0.0%	0.0%
Diethyl N-[4-(4-oxobutyl)benzoyl]-L-glutamate	608-229-3	2863-88-9	2863889	2540	Reach_4266	3486	3.00	0.81	3				-6.6	-7.2	-8.7	0.0%	0.0%	0.0%
betahistine	609-695-0	394735-17-2	394735172	2840	Reach_4307	3487	4.36	0.78	3				-7.4	-7.2	-8.3	0.0%	0.0%	0.0%
600-553-3	222-111-5	3351-05-1	3351051	1183	Reach_1952	3488	3.64		1				-6.7	-7.2	-8.5	0.0%	0.0%	0.0%
isovaleryl chloride	218-485-4	2162-73-4	2162734	2299	Reach_1766	3489	5.50	1.16	3	4.26	1.84		-7.4	-7.2	-8.9	0.0%	0.0%	0.0%
fluocortolone	806-511-2	35877-42-0	35877420	2753	Reach_5074	3490	3.46	0.78	3				-6.5	-7.2	-8.7	0.0%	0.0%	0.0%
618-883-1	617-590-6	846023-24-3	846023243	3869	Reach_4469	3491	4.11		1				-7.2	-7.2	-8.7	0.0%	0.0%	0.0%
606-376-8	609-972-6	41965-95-1	41965951	5883	Reach_4318	3492							-6.5	-7.2	-8.7	0.0%	0.0%	0.0%
3-benzylidenephthalide	610-717-6	5173-46-6	5173466	3045	Reach_4334	3493	4.51	0.22	3				-7.0	-7.2	-8.7	0.0%	0.0%	0.0%
613-901-4	613-901-4	6615-00-5	6615005	3465	Reach_4389	3494	4.77		2				-6.4	-7.2	-8.9	0.0%	0.0%	0.0%
o-phenethylbenzoic acid	218-121-4	2051-49-2	2051492	2270	Reach_1753	3495	4.73		1				-6.8	-7.2	-8.7	0.0%	0.0%	0.0%
5-bromo-2-nitropyridine	210-088-4	605-50-5	605505	3311	Reach_1413	3496	2.67	0.31	3				-7.4	-7.2	-8.7	0.0%	0.0%	0.0%
5'-chloro-3-hydroxy-2',4'-dimethoxy-2-naphthanilide	202-182-9	92-72-8	92728	4047	Reach_390	3497	2.84	0.25	3				-6.6	-7.2	-8.6	0.0%	0.0%	0.0%
2-chloro-3-(hydroxymethylene)cyclohex-1-ene-1-carbaldehyde	615-113-6	704-10-9	704109	3562	Reach_4409	3498	2.40	2.37	3				-6.7	-7.2	-8.7	0.0%	0.0%	0.0%
N-[3-({[2,2-dimethyl-3-(morpholin-4-yl)propylidene]amino}meth	700-584-3	1217271-02-7	1217271027	1735	Reach_4940	3499	4.53		2				-6.7	-7.2	-8.5	0.0%	0.0%	0.0%
4-[(4-chloropyrimidin-2-yl)amino]benzonitrile	607-384-4	244768-32-9	244768329	2396	Reach_4240	3500	4.14	0.60	3				-6.7	-7.2	-8.7	0.0%	0.0%	0.0%
3-(vinyloxy)propan-1-amine	700-340-6	76524-94-2	76524942	3715	Reach_4868	3501	5.03	0.86	3	4.03	0.86		-7.4	-7.2	-8.7	0.0%	0.0%	0.0%
benzidine-2,2'-disulphonic acid	204-179-8	117-21-5	117215	1657	Reach_958	3502	6.42	0.29	3	5.42	0.29		-6.1	-7.2	-8.9	0.0%	0.0%	0.0%
620-466-4	284-362-7	84852-49-3	84852493	6055	Reach_2981	3503	5.41	1.21	3	4.39	1.46		-6.4	-7.2	-8.8	0.0%	0.0%	0.0%
3-aminopyrazine-2-carboxylic acid	226-558-7	5424-01-1	5424011	1275	Reach_2111	3504	4.39	1.02	3				-6.4	-7.2	-8.8	0.0%	0.0%	0.0%
617-350-0	617-350-0	82543-18-8	82543188	3831	Reach_4457	3505	4.71		1				-6.5	-7.2	-8.7	0.0%	0.0%	0.0%
mesterolone	253-258-3	36894-69-6	36894696	2785	Reach_2707	3506	3.66	0.40	3				-6.7	-7.2	-8.7	0.0%	0.0%	0.0%
methyl phenylacetate	601-621-5	119532-26-2	119532262	5623	Reach_4096	3507	3.21		1				-7.4	-7.2	-8.7	0.0%	0.0%	0.0%
methyl ({[(1Z)-1-(2-amino-1,3-thiazol-4-yl)-2-(1,3-benzothiazol-2-	204-344-4	119-70-0	119700	1698	Reach_985	3508	5.01		1				-6.7	-7.2	-8.9	0.0%	0.0%	0.0%
2-(6-hydroxy-3-oxo-(3H)-xanthen-9-yl)benzoic acid	700-492-3	1207628-34-9	1207628349	1720	Reach_4912	3509	4.56	0.97	3				-6.5	-7.2	-8.7	0.0%	0.0%	0.0%
perfluoroethane	200-004-4	50-03-3	50033	2995	Reach_3	3510	4.32	0.67	3				-7.5	-7.2	-9.5	0.0%	0.0%	0.0%
3-methylpentan-2-one	222-102-6	3349-08-4	3349084	5580	Reach_1951	3511							-7.4	-7.2	-8.6	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
colchicine	200-598-5	64-86-8	64868	782	Reach_75	3512	5.70		1	5.00			-6.6	-7.2	-8.6	0.0%	0.0%	0.0%
allyl heptanoate	205-527-1	142-19-8	142198	1950	Reach_1174	3513	2.97	0.65	3	2.11	0.52		-7.4	-7.2	-8.8	0.0%	0.0%	0.0%
methyl p-toluate	202-784-1	99-75-2	99752	4215	Reach_537	3514	3.98	0.87	3	2.98	0.87		-7.4	-7.2	-8.4	0.0%	0.0%	0.0%
boldenone	212-686-0	846-48-0	846480	3873	Reach_1566	3515	4.67		2				-6.7	-7.2	-8.7	0.0%	0.0%	0.0%
2-phenylethyl 2-cyanoacrylate	633-172-6	66415-55-2	66415552	3472	Reach_4600	3516	4.58		1				-7.4	-7.2	-8.8	0.0%	0.0%	0.0%
(6α,9β,11β,16α)-6-fluoro-17-hydroxy-16-methyl-3,20-dioxo-9,11	700-111-0	148528-05-6	148528056	2002	Reach_4767	3517	4.72	0.18	3	3.72	0.18		-6.6	-7.2	-8.7	0.0%	0.0%	0.0%
[4-(2-chloroethoxy)phenyl](phenyl)methanone	613-733-1	64987-06-0	64987060	3447	Reach_4386	3518	4.62	1.36	3				-7.4	-7.2	-8.8	0.0%	0.0%	0.0%
3,3'-[methylenebis(oxymethylene)]bisheptane	700-823-1	55514-22-2	55514222	3171	Reach_5002	3519	-0.76	1.61	3				-7.4	-7.2	-8.3	0.0%	0.0%	0.0%
1,3,5-triisopropylbenzene	231-472-8	7575-23-7	7575237	3684	Reach_2261	3520	2.79	0.62	3	1.79	0.62		-7.4	-7.2	-9.3	0.0%	0.0%	0.0%
trimethylsilyl undec-10-enoate	606-964-4	222408-90-4	222408904	2324	Reach_4230	3521	3.25	0.64	3				-7.4	-7.2	-8.8	0.0%	0.0%	0.0%
pentan-2-one	203-528-1	107-87-9	107879	223	Reach_717	3522	5.81	0.60	3	4.81	0.60		-7.4	-7.2	-8.5	0.0%	0.0%	0.0%
3,4,5-trimethoxybenzoic acid	202-000-8	90-51-7	90517	4001	Reach_365	3523	4.89	0.70	3	3.89	0.70		-6.5	-7.2	-8.9	0.0%	0.0%	0.0%
1,2,2,6,6-pentamethylpiperidin-4-ol	201-879-5	89-05-4	89054	3968	Reach_338	3524	4.23		2				-7.3	-7.2	-8.8	0.0%	0.0%	0.0%
decyl methacrylate	221-657-1	3179-47-3	3179473	2635	Reach_1927	3525	3.46	1.77	3	2.46	1.77		-7.4	-7.2	-8.7	0.0%	0.0%	0.0%
N-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfan	601-485-7	117570-93-1	117570931	1660	Reach_4090	3526	3.89	0.30	3				-6.6	-7.2	-8.7	0.0%	0.0%	0.0%
Benzyl N-(2-benzylacryloyl)glycinate	700-731-1	35958-64-6	35958646	2755	Reach_4980	3527	3.97	0.34	3				-6.7	-7.2	-8.8	0.0%	0.0%	0.0%
diethyl diallylmalonate	262-475-2	60857-05-8	60857058	3318	Reach_2847	3528	4.52		1				-7.5	-7.2	-8.6	0.0%	0.0%	0.0%
Dilithium naphthalene-1,5-disulfonate	700-037-9	152845-00-6	152845006	5712	Reach_4734	3529	4.86		1				-7.0	-7.2	-8.6	0.0%	0.0%	0.0%
butamirate	230-467-8	7148-78-9	7148789	3583	Reach_2227	3530	1.13	4.54	3				-7.4	-7.2	-8.8	0.0%	0.0%	0.0%
1,1,2,3,3-pentamethylindan	607-173-7	22871-58-5	22871585	2340	Reach_4234	3531	5.46	0.24	3	4.46	0.24		-7.5	-7.2	-8.9	0.0%	0.0%	0.0%
619-422-7	217-504-3	1874-83-5	1874835	5750	Reach_1729	3532							-7.5	-7.2	-8.9	0.0%	0.0%	0.0%
(4,5-dibromo-1H-pyrrol-2-yl)(phenyl)methanone	211-490-2	652-37-9	652379	3448	Reach_1487	3533	4.61	1.38	3				-7.4	-7.2	-8.8	0.0%	0.0%	0.0%
3,3'-[biphenyl-4,4'-diylbis(oxy)]dianiline	700-102-1	105112-76-3	105112763	1409	Reach_4764	3534	2.83	0.34	3				-6.7	-7.3	-8.8	0.0%	0.0%	0.0%
2-methylpent-2-enal	696-106-5	1176987-11-3	1176987113	5616	Reach_4704	3535							-7.5	-7.3	-8.5	0.0%	0.0%	0.0%
dioctylamine	214-311-6	1120-48-5	1120485	1570	Reach_1658	3536	1.99		2				-7.4	-7.3	-9.0	0.0%	0.0%	0.0%
(2-isobutyl-2-methyl-1,3-dioxolan-4-yl)methanol	616-639-9	78620-07-2	78620072	6037	Reach_4441	3537	5.36		1				-7.4	-7.3	-8.8	0.0%	0.0%	0.0%
4-[2-(Dimethylamino)-1-(1-hydroxycyclohexyl)ethyl]phenol	700-299-4	2896-97-1	2896971	2551	Reach_4850	3538	2.90	0.50	3				-6.6	-7.3	-8.8	0.0%	0.0%	0.0%
Tetrasodium {3,3',3'',3'''-[(29H,31H-phthalocyanine-1,8,15,22-te	696-145-8	944730-39-6	944730396	6091	Reach_4707	3539	5.16	0.58	3	4.16	0.58		-7.0	-7.3	-8.6	0.0%	0.0%	0.0%
allyl 2-hydroxy-2-methylpropanoate	700-908-3	19444-21-4	19444214	2233	Reach_5024	3540	4.14	0.46	3	3.14	0.46		-7.4	-7.3	-8.9	0.0%	0.0%	0.0%
3-hydroxy-4-[(2-methyl-4-nitrophenyl)azo]-N-(o-tolyl)naphthale	211-383-0	642-31-9	642319	3431	Reach_1479	3541	2.84	0.33	3				-7.1	-7.3	-7.9	0.0%	0.0%	0.0%
3-methoxyoestra-1,3,5(10)-trien-17-one	217-968-7	2022-85-7	2022857	2255	Reach_1745	3542	4.77	1.48	3				-7.4	-7.3	-8.8	0.0%	0.0%	0.0%
601-431-2	700-505-2	37486-69-4	37486694	2799	Reach_4914	3543							-7.3	-7.3	-8.7	0.0%	0.0%	0.0%
L-cysteine	200-158-2	52-90-4	52904	3080	Reach_18	3544	5.50		3	4.50			-6.2	-7.3	-9.0	0.0%	0.0%	0.0%
3-hydroxybenzaldehyde	604-453-0	145022-45-3	145022453	5700	Reach_4154	3545	4.62		2				-7.3	-7.3	-8.8	0.0%	0.0%	0.0%
607-977-8	607-985-1	26678-02-4	26678024	2483	Reach_4257	3546	5.81		1				-7.5	-7.3	-9.5	0.0%	0.0%	0.0%
2-methylbutyl acrylate	256-170-3	44914-03-6	44914036	2934	Reach_2755	3547	3.57	0.33	3	2.91	0.21		-7.5	-7.3	-8.8	0.0%	0.0%	0.0%
2-Methyloctane-1,8-diamine	700-023-2	130198-05-9	130198059	5658	Reach_4118	3548							-7.5	-7.3	-8.7	0.0%	0.0%	0.0%
610-141-5	610-141-5	437717-43-6	437717436	2915	Reach_4322	3549	3.69	1.01	3				-6.4	-7.3	-8.8	0.0%	0.0%	0.0%
N-phenylacrylamide	606-936-1	2210-24-4	2210244	2318	Reach_4225	3550	4.62		1				-7.3	-7.3	-8.8	0.0%	0.0%	0.0%
5-amino-2-(p-aminoanilino)benzenesulphonic acid	700-101-6	246035-38-1	246035381	2399	Reach_4763	3551	2.74	0.29	3				-6.3	-7.3	-8.9	0.0%	0.0%	0.0%
tert-butyl 4-(6-aminopyridin-3-yl)piperazine-1-carboxylate	695-268-4	571188-59-5	571188595	3224	Reach_4691	3552	3.90	0.87	3				-6.7	-7.3	-8.8	0.0%	0.0%	0.0%
ethyl (2Z)-4,4,4-trifluoro-3-(methylamino)but-2-enoate	687-796-9	1254333-41-9	1254333419	5642	Reach_4639	3553							-7.4	-7.3	-8.9	0.0%	0.0%	0.0%
N-{6-[3-tert-butyl-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-2-	805-439-9	1132935-63-7	1132935637	1615	Reach_5065	3554	2.49	0.24	3				-6.7	-7.3	-8.7	0.0%	0.0%	0.0%
5-aminosalicylic acid	299-135-8	93857-00-2	93857002	6085	Reach_3002	3555	6.31	0.30	3	5.31	0.30		-6.5	-7.3	-8.9	0.0%	0.0%	0.0%
603-982-4	603-982-4	136890-21-6	136890216	1904	Reach_4136	3556	1.28	0.71	3				-6.9	-7.3	-8.1	0.0%	0.0%	0.0%
1,2,3,4-tetrahydro-1,1,2,4,4,7-hexamethylnaphthalene	619-692-6	156366-26-6	156366266	2047	Reach_4536	3557	3.04	0.51	3				-7.5	-7.3	-8.7	0.0%	0.0%	0.0%
(3,3-diethoxy-1-propenyl)benzene	204-333-4	119-56-2	119562	1695	Reach_980	3558	3.42	0.48	3				-7.5	-7.3	-8.8	0.0%	0.0%	0.0%
611-631-1	611-631-1	58190-57-1	58190571	3242	Reach_4363	3559	5.57	0.27	3	4.57	0.27		-7.1	-7.3	-8.0	0.0%	0.0%	0.0%
1-(2-chloroethoxy)-4-(1,2-diphenylvinyl)benzene	700-227-1	40722-73-4	40722734	2862	Reach_4812	3560	4.72	1.30	3				-7.1	-7.3	-8.4	0.0%	0.0%	0.0%
2-hexyldecyl methanesulfonate	212-985-6	901-44-0	901440	3991	Reach_1588	3561	4.24	0.45	3	3.24	0.45		-7.6	-7.3	-9.4	0.0%	0.0%	0.0%
615-927-1	609-206-0	361366-16-7	361366167	2759	Reach_4294	3562	3.10	0.37	3				-7.5	-7.3	-9.0	0.0%	0.0%	0.0%
trimethylsilyl N-trimethylsilylacetamidate	225-063-3	4637-24-5	4637245	2953	Reach_2052	3563	7.42	0.67	3	6.42	0.67		-7.5	-7.3	-9.7	0.0%	0.0%	0.0%
ethyl N-(diphenylmethylidene)glycinate	614-987-6	69555-14-2	69555142	3544	Reach_4405	3564	3.23	0.17	3				-6.9	-7.3	-8.9	0.0%	0.0%	0.0%
phenyl diamidophosphate	231-218-6	7450-69-3	7450693	3638	Reach_2251	3565	4.31		2				-6.5	-7.3	-9.1	0.0%	0.0%	0.0%
1-methylhexyl chloroacetate	606-870-3	219715-34-1	219715341	2312	Reach_4222	3566	4.97		1				-7.5	-7.3	-8.7	0.0%	0.0%	0.0%
3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulphonyl chloride	610-147-8	438056-69-0	438056690	2917	Reach_4323	3567	3.95		1				-7.5	-7.3	-9.7	0.0%	0.0%	0.0%
benzyl (4-bromo-3-fluorophenyl)carbamate	265-250-7	64838-55-7	64838557	3444	Reach_2867	3568	4.78	1.41	3				-7.5	-7.3	-8.8	0.0%	0.0%	0.0%
tert-pentyl 2-ethylperoxyhexanoate	211-687-3	686-31-7	686317	3523	Reach_1502	3569	2.81		2				-7.5	-7.3	-9.6	0.0%	0.0%	0.0%
1,1,1,2,4,4,5,7,7,8,10,10,11,13,13,14,16,16,17,17,18,18,18-tricos	228-771-0	6358-37-8	6358378	3408	Reach_2169	3570	5.26	1.21	3	4.26	1.21		-7.5	-7.3	-8.0	0.0%	0.0%	0.0%
diethyl (phenylmethylene)malonate	266-330-4	66356-53-4	66356534	3470	Reach_2878	3571	4.22	0.81	3				-7.5	-7.3	-8.8	0.0%	0.0%	0.0%
but-3-enenitrile	203-701-1	109-75-1	109751	264	Reach_789	3572	5.26		2				-7.5	-7.3	-8.4	0.0%	0.0%	0.0%
O-(2-ethylhexyl) O,O-tert-pentyl peroxycarbonate	274-919-2	70833-40-8	70833408	3570	Reach_2921	3573	2.75	0.05	3				-7.5	-7.3	-8.7	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
ethyl 2-methylvalerate	204-688-5	124-19-6	124196	1788	Reach_1073	3574	3.35	0.18	3	2.47	0.19		-7.6	-7.3	-8.9	0.0%	0.0%	0.0%
4-[(4,6-Bis{[3-(diethylamino)propyl]amino}-1,3,5-triazin-2-yl)ami	700-650-1	909782-35-0	909782350	4010	Reach_4959	3575	2.44		1				-7.3	-7.3	-7.7	0.0%	0.0%	0.0%
myristoyl chloride	800-308-2	1160221-25-9	1160221259	1641	Reach_5044	3576	2.15	0.86	3				-7.6	-7.3	-9.5	0.0%	0.0%	0.0%
3-(9,10-ethano-9(10H)-anthryl)acrylaldehyde	226-529-9	5419-55-6	5419556	3131	Reach_2108	3577							-7.5	-7.3	-8.8	0.0%	0.0%	0.0%
601-507-5	226-845-7	5505-16-8	5505168	3158	Reach_2119	3578	3.74	0.67	3				-7.6	-7.3	-9.7	0.0%	0.0%	0.0%
ethyl [(1-chloro-10-oxo-10H-dibenzo[b,e]thiopyran-4-yl)oxy]acet	700-766-2	61010-04-6	61010046	3323	Reach_4988	3579	3.83	1.74	3				-7.1	-7.3	-8.8	0.0%	0.0%	0.0%
icosanoic acid	209-935-0	598-50-5	598505	3289	Reach_1402	3580	4.84	1.66	3				-7.3	-7.3	-8.5	0.0%	0.0%	0.0%
1-(2-ethylbutyl)cyclohexanecarbonyl chloride	259-515-6	55184-72-0	55184720	5929	Reach_2806	3581	3.99	0.72	3	2.99	0.72		-7.6	-7.3	-9.5	0.0%	0.0%	0.0%
608-211-5	608-211-5	284462-37-9	284462379	2532	Reach_4265	3582	4.46		2				-6.6	-7.3	-9.0	0.0%	0.0%	0.0%
N,N'-[cyclohexane-1,3-diylbis(methylene)]bis(2-methylpropan-1·	619-764-7	173904-11-5	173904115	2133	Reach_4543	3583	4.48	0.34	3	3.63	0.34		-7.5	-7.3	-8.3	0.0%	0.0%	0.0%
614-960-9	614-960-9	69399-57-1	69399571	3542	Reach_4403	3584	5.19	1.05	3				-6.3	-7.3	-9.1	0.0%	0.0%	0.0%
(4S)-4-(phenylthio)-L-proline	202-215-7	93-07-2	93072	4058	Reach_398	3585	4.18	0.62	3				-6.3	-7.3	-9.0	0.0%	0.0%	0.0%
3-nitro-p-anisic acid	201-906-0	89-41-8	89418	3975	Reach_343	3586	5.24	0.74	3				-6.7	-7.3	-9.1	0.0%	0.0%	0.0%
benzimidazole-2-thiol	200-984-3	76-75-5	76755	877	Reach_177	3587	4.42		1				-6.6	-7.3	-9.0	0.0%	0.0%	0.0%
calcium bis{4-[(E)-(5-carbamoyl-2-methoxyphenyl)diazenyl]-3-hy	700-038-4	17273-79-9	17273799	5739	Reach_4735	3588							-7.1	-7.3	-8.7	0.0%	0.0%	0.0%
604-604-0	252-677-9	35689-59-9	35689599	5857	Reach_2693	3589							-6.9	-7.3	-8.7	0.0%	0.0%	0.0%
Ethyl 3-cyclobutylalaninate	227-086-4	5638-76-6	5638766	3195	Reach_2130	3590	4.12	0.88	3				-7.5	-7.3	-8.9	0.0%	0.0%	0.0%
5-chlorothiophene-2-sulfonamide	805-591-6	210223-97-5	210223975	5770	Reach_5066	3591							-6.7	-7.3	-8.9	0.0%	0.0%	0.0%
806-599-2	680-297-7	88110-89-8	88110898	3947	Reach_4624	3592	4.25	1.42	3				-6.9	-7.3	-8.8	0.0%	0.0%	0.0%
Sodium naphthalene-2-carboxylate	700-756-8	1204232-63-2	1204232632	5626	Reach_4986	3593							-7.1	-7.3	-8.7	0.0%	0.0%	0.0%
1-{[(methylsulfanyl)carbonyl]oxy}ethyl 2-methylpropanoate	700-047-3	860035-07-0	860035070	3899	Reach_4739	3594	4.42	0.95	3				-7.5	-7.4	-8.8	0.0%	0.0%	0.0%
610-977-0	700-391-4	6953-28-2	6953282	6003	Reach_4885	3595							-6.7	-7.4	-8.7	0.0%	0.0%	0.0%
1-(1,1-dimethylethoxy)-2-methylpropane	212-811-9	871-78-3	871783	3920	Reach_1577	3596	5.20	1.69	3				-7.6	-7.4	-9.7	0.0%	0.0%	0.0%
3-(2-(2-Hydroxyethoxy)ethylimino)-2,2-dimethylpropyldodecanc	700-067-2	931419-77-1	931419771	4062	Reach_4748	3597	4.30		2				-6.8	-7.4	-8.9	0.0%	0.0%	0.0%
methyl 3-oxohexanoate	213-493-4	959-14-8	959148	4137	Reach_1618	3598	3.39	0.61	3				-7.5	-7.4	-8.7	0.0%	0.0%	0.0%
(2S,3S,5R)-3-methyl-7-oxo-3-(1H-1,2,3-triazol-1-ylmethyl)-4-thia·	618-303-7	89786-04-9	89786049	3986	Reach_4492	3599	6.24	2.11	3				-6.3	-7.4	-9.0	0.0%	0.0%	0.0%
610-200-5	700-255-4	31775-89-0	31775890	2633	Reach_4825	3600	2.91	1.30	3	1.91	1.30		-6.4	-7.4	-9.0	0.0%	0.0%	0.0%
diisopentyl ether	208-857-4	544-01-4	544014	3141	Reach_1351	3601	3.78	0.28	3	2.78	0.28		-7.6	-7.4	-9.5	0.0%	0.0%	0.0%
619-847-8	619-847-8	111298-82-9	111298829	1546	Reach_4550	3602	4.52	0.65	3				-6.5	-7.4	-8.9	0.0%	0.0%	0.0%
N-(5-chloro-2,4-dimethoxyphenyl)-4-[[5-[(diethylamino)sulphony	229-107-2	6410-41-9	6410419	3425	Reach_2179	3603	5.04	1.10	3	4.04	1.10		-7.0	-7.4	-8.2	0.0%	0.0%	0.0%
methyl hexanoate	239-263-3	15206-55-0	15206550	2020	Reach_2377	3604	4.39	0.94	3				-7.6	-7.4	-9.0	0.0%	0.0%	0.0%
octafluoropropane	200-941-9	76-19-7	76197	3702	Reach_174	3605	4.32	0.19	3				-7.6	-7.4	-9.6	0.0%	0.0%	0.0%
N-(4-{[3-(dimethylamino)propyl]sulfamoyl}phenyl)-2-[(2-methox	700-222-4	1065519-44-9	1065519449	1438	Reach_4809	3606	0.93		1				-6.7	-7.4	-8.8	0.0%	0.0%	0.0%
607-088-5	607-088-5	224785-90-4	224785904	2334	Reach_4232	3607	3.50	0.93	3				-6.8	-7.4	-8.8	0.0%	0.0%	0.0%
bis(2-propylheptyl) carbonate	700-195-9	223398-24-1	223398241	5782	Reach_4800	3608							-7.3	-7.4	-8.6	0.0%	0.0%	0.0%
cyclopentene	700-377-8	99817-37-5	99817375	4217	Reach_4882	3609	3.20	0.29	3				-7.6	-7.4	-9.8	0.0%	0.0%	0.0%
2,3-Dihydro-1,4-benzodioxin-2-yl(piperazin-1-yl)methanone	685-040-2	81778-06-5	81778065	3812	Reach_4629	3610	4.48	1.35	3				-6.6	-7.4	-9.1	0.0%	0.0%	0.0%
6-[3-tert-butyl-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-2-me	695-991-5	1355646-97-7	1355646977	1890	Reach_4700	3611	1.01	0.60	3				-7.2	-7.4	-7.9	0.0%	0.0%	0.0%
menthyl acetate	201-911-8	89-48-5	89485	3976	Reach_344	3612	3.82	0.64	3	2.98	0.74		-7.6	-7.4	-8.8	0.0%	0.0%	0.0%
2-ethylhexyl nonanoate	700-472-4	27665-39-0	27665390	2514	Reach_4906	3613	7.22	0.66	3				-7.5	-7.4	-8.9	0.0%	0.0%	0.0%
methyl L-threoninate	608-135-2	27710-82-3	27710823	5811	Reach_4261	3614							-7.0	-7.4	-9.2	0.0%	0.0%	0.0%
3,5-bis(2,4-dimethylcyclohex-3-en-1-yl)dihydro-1H-[1,3]oxazolo[	700-437-3	1196069-20-1	1196069201	1696	Reach_4899	3615	3.05		1				-7.2	-7.4	-8.7	0.0%	0.0%	0.0%
ethyl trichloroacetate	208-212-7	515-84-4	515844	3042	Reach_1320	3616	4.90	0.28	3	3.90	0.28		-7.6	-7.4	-9.0	0.0%	0.0%	0.0%
1-(2,4-dichloro-5-fluorophenyl)ethanone	256-127-9	43170-88-3	43170883	2906	Reach_2754	3617	4.93	1.10	3				-7.6	-7.4	-8.5	0.0%	0.0%	0.0%
1-chlorohexane	245-485-1	23202-81-5	23202815	2347	Reach_2528	3618	5.88	0.45	3				-7.7	-7.4	-9.7	0.0%	0.0%	0.0%
diisopentyl phthalate	678-536-5	52698-46-1	52698461	3070	Reach_4619	3619	5.00	0.59	3				-7.1	-7.4	-8.8	0.0%	0.0%	0.0%
tetrachloro-1,2-difluoroethane	200-935-6	76-12-0	76120	3700	Reach_172	3620	3.97	0.13	3				-7.8	-7.4	-9.6	0.0%	0.0%	0.0%
trifluoroacetic anhydride	206-982-9	407-25-0	407250	2863	Reach_1267	3621	6.01	1.57	3	5.01	1.57		-7.7	-7.4	-10.1	0.0%	0.0%	0.0%
5-amino-3-methylthiophene-2,4-dicarbonitrile	269-389-4	68227-78-1	68227781	3512	Reach_2902	3622	5.04	1.10	3	4.04	1.10		-6.8	-7.4	-9.1	0.0%	0.0%	0.0%
N-(2-Bromo-5-hydroxy-4-methoxybenzyl)-N-[2-(4-hydroxypheny	602-791-3	122584-18-3	122584183	1753	Reach_4105	3623	3.46	0.30	3				-6.8	-7.4	-9.0	0.0%	0.0%	0.0%
(3R)-3-[2-(Benzyloxy)-5-bromophenyl]-N,N-diisopropyl-3-phenylp	604-958-6	15448-47-2	15448472	489	Reach_4165	3624	4.86	0.38	3				-7.1	-7.4	-8.1	0.0%	0.0%	0.0%
(2-formamido-1,3-thiazol-4-yl)(oxo)acetic acid	690-635-5	3439-73-4	3439734	2703	Reach_4658	3625	3.46	0.19	3				-6.5	-7.4	-9.1	0.0%	0.0%	0.0%
689-979-9	689-979-9	116817-12-0	116817120	5613	Reach_4655	3626							-7.2	-7.4	-8.8	0.0%	0.0%	0.0%
pentyl propionate	217-775-8	1951-97-9	1951979	5761	Reach_1738	3627	5.61	0.80	3	4.61	0.80		-7.7	-7.4	-9.0	0.0%	0.0%	0.0%
1-Phenylsulfonylpyrrole	623-685-3	16851-82-4	16851824	2113	Reach_4578	3628	3.84	0.88	3				-6.8	-7.4	-9.1	0.0%	0.0%	0.0%
(S)-p-mentha-1,8-diene	227-815-6	5989-54-8	5989548	744	Reach_2148	3629	3.96	0.91	7	2.96	0.91		-7.7	-7.4	-9.7	0.0%	0.0%	0.0%
triacetoxyvinylsilane	223-943-1	4130-08-9	4130089	1265	Reach_2015	3630	5.64	0.92	3	4.64	0.51		-7.5	-7.4	-9.1	0.0%	0.0%	0.0%
2-chloro-1-(3,4-difluorophenyl)ethanone	607-988-8	2668-75-9	2668759	2484	Reach_4258	3631	3.70		2				-7.7	-7.4	-8.7	0.0%	0.0%	0.0%
(Z)-hex-3-enyl acetate	222-960-1	3681-71-8	3681718	2779	Reach_1979	3632	4.55	0.33	3	3.86	0.28		-7.7	-7.4	-9.0	0.0%	0.0%	0.0%
1-[3-tert-butyl-5-(6-hydroxy-2-naphthyl)-4-methoxyphenyl]pyrin	805-127-2	1355646-93-3	1355646933	1889	Reach_5061	3633	2.18	0.17	3				-6.8	-7.4	-8.7	0.0%	0.0%	0.0%
1-(benzyloxy)-4-[2-(cyclopropylmethoxy)ethyl]benzene	613-114-6	62932-92-7	62932927	3388	Reach_4381	3634	2.24	0.78	3				-7.5	-7.4	-8.8	0.0%	0.0%	0.0%
602-769-3	700-172-3	634-55-9	634559	3402	Reach_4789	3635	4.75		2				-6.5	-7.4	-9.2	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
thiocolchicine	220-346-8	2730-71-4	2730714	2499	Reach_1859	3636	3.08	0.53	3				-6.9	-7.5	-8.9	0.0%	0.0%	0.0%
3-amino-4-hydroxybenzenesulphonic acid	256-442-1	49715-04-0	49715040	2988	Reach_2764	3637	4.72	1.22	3				-6.5	-7.5	-9.3	0.0%	0.0%	0.0%
1,1,3,3-tetramethylbutyl 2-ethylperoxyhexanoate	244-894-2	22288-43-3	22288433	2328	Reach_2521	3638	4.97		1				-7.6	-7.5	-9.0	0.0%	0.0%	0.0%
L-leucine	700-811-6	87428-99-7	87428997	3934	Reach_5000	3639	3.30	0.67	3				-6.4	-7.5	-9.1	0.0%	0.0%	0.0%
2,2-Dimethyl-3-(morpholin-4-yl)propanal	700-569-1	23588-51-4	23588514	2352	Reach_4937	3640	4.51	0.80	3				-7.0	-7.5	-9.2	0.0%	0.0%	0.0%
5-methylisoxazole-4-carboxylic acid	700-843-0	198979-98-5	198979985	6399	Reach_5008	3641							-6.7	-7.5	-9.1	0.0%	0.0%	0.0%
Cyclopropane-1,1-diyldimethanol	700-582-2	30392-50-8	30392508	5831	Reach_4939	3642	3.70		1				-7.0	-7.5	-9.2	0.0%	0.0%	0.0%
(R)-quinuclidin-3-ol	610-977-0	53201-62-0	53201620	3090	Reach_4342	3643	3.17	0.80	3				-6.7	-7.5	-9.2	0.0%	0.0%	0.0%
piperidine-2-methylamine	700-696-2	1062580-52-2	1062580522	5597	Reach_4971	3644							-7.4	-7.5	-9.2	0.0%	0.0%	0.0%
4-methoxybenzyl (6R,7R)-7-amino-3-(chloromethyl)-8-oxo-5-thia	800-008-1	21524-36-7	21524367	2296	Reach_5034	3645	3.07	0.65	3				-6.4	-7.5	-9.2	0.0%	0.0%	0.0%
N-(2-ethylhexyl)isononan-1-amide	806-533-2	1219086-87-9	1219086879	1738	Reach_5075	3646	2.42	0.04	3				-7.6	-7.5	-8.6	0.0%	0.0%	0.0%
(5,6-Dimethyl-9-oxo-9H-xanthen-4-yl)acetic acid	696-006-1	123348-27-6	123348276	1769	Reach_4703	3647	2.56	0.27	3				-7.0	-7.5	-9.1	0.0%	0.0%	0.0%
609-736-2	204-975-5	130-13-2	130132	5657	Reach_1116	3648	6.45		1				-6.7	-7.5	-9.0	0.0%	0.0%	0.0%
2-methylquinoline-4-carboxamide	239-917-8	15821-13-3	15821133	2058	Reach_2400	3649	3.98	1.08	3				-6.8	-7.5	-9.1	0.0%	0.0%	0.0%
retinyl acetate	204-844-2	127-47-9	127479	1812	Reach_1098	3650	3.42	1.01	3	2.57	1.08		-7.2	-7.5	-8.2	0.0%	0.0%	0.0%
S-1,3-benzothiazol-2-yl (2Z)-(2-amino-1,3-thiazol-4-yl)[(trityloxy)i	606-000-2	1836-62-0	1836620	2186	Reach_4189	3651	4.26	0.83	3				-7.0	-7.5	-8.9	0.0%	0.0%	0.0%
2-[3-(9-butyl-1,1,3,3,5,5,7,7,9,9-decamethylpentasiloxanyl)propo	801-072-3	1052075-57-6	1052075576	1411	Reach_5051	3652	0.11	1.74	3				-7.7	-7.5	-8.1	0.0%	0.0%	0.0%
610-201-0	610-200-5	446292-07-5	446292075	2929	Reach_4326	3653	4.65	1.21	3				-6.7	-7.5	-9.1	0.0%	0.0%	0.0%
3-Hydroxy-2,2-dimethyl-N-propylpropanamide	219-351-8	2422-91-5	2422915	2380	Reach_1804	3654	5.50		3	4.50			-6.5	-7.5	-9.1	0.0%	0.0%	0.0%
2,2,6,6-Tetramethylpiperidin-4-yl dodecanoate	700-503-1	101238-01-1	101238011	1317	Reach_4913	3655	2.51	0.40	3	1.47	0.66		-7.4	-7.5	-8.6	0.0%	0.0%	0.0%
3-amino-4-methoxybenzenesulphonic acid	609-812-5	402913-84-2	402913842	2856	Reach_4313	3656	4.59	1.57	3				-6.6	-7.5	-9.2	0.0%	0.0%	0.0%
610-472-5	610-472-5	49707-23-5	49707235	2987	Reach_4329	3657	4.45	0.52	3				-6.5	-7.5	-9.1	0.0%	0.0%	0.0%
gestonorone	700-845-1	133978-15-1	133978151	1874	Reach_5009	3658	3.23	0.27	3				-6.8	-7.5	-9.0	0.0%	0.0%	0.0%
2,5-bis(2,2,2-trifluoroethoxy)benzoic acid	611-756-1	58861-48-6	58861486	3255	Reach_4364	3659	3.47	0.12	3				-6.9	-7.5	-9.2	0.0%	0.0%	0.0%
(2β,3α,5α,16β,17β)-2-(morpholin-4-yl)-16-(pyrrolidin-1-yl)andros	205-812-0	153-00-4	153004	2027	Reach_1210	3660	4.06	0.26	3				-6.8	-7.5	-9.0	0.0%	0.0%	0.0%
3,3,4,4,5,5,6,6,6-nonafluorohexene	243-053-7	19430-93-4	19430934	2231	Reach_2479	3661	3.65	0.14	3	2.65	0.14		-7.8	-7.5	-10.2	0.0%	0.0%	0.0%
3-(3,5-di-tert-butyl-4-hydroxyphenyl)-N-octadecylpropanamide	700-596-9	14442-94-5	14442945	1976	Reach_4944	3662	1.30	0.25	3	0.30	0.25		-7.7	-7.5	-7.9	0.0%	0.0%	0.0%
(S)-1-[3-(acetylthio)-2-methyl-1-oxopropyl]-L-proline	609-612-8	3910-51-8	3910518	2834	Reach_4306	3663	2.89	0.06	3				-6.6	-7.5	-9.2	0.0%	0.0%	0.0%
2,4-dihydroxybenzophenone	205-029-4	131-56-6	131566	1850	Reach_1121	3664	3.60	0.29	3	2.60	0.29		-7.0	-7.5	-9.0	0.0%	0.0%	0.0%
2-oxopropyl 3-(benzyl-[4-(2-cyano-4-nitrophenylazo)phenyl]amir	627-085-2	1238449-42-7	1238449427	1776	Reach_4584	3665	5.33	0.25	3	4.33	0.25		-7.0	-7.5	-9.2	0.0%	0.0%	0.0%
1,1,1,2,2,3,3,4,5,5,5-undecafluoro-4-(trifluoromethyl)pentane	206-575-6	355-04-4	355044	2740	Reach_1250	3666	3.10	0.25	3				-7.8	-7.5	-9.7	0.0%	0.0%	0.0%
600-715-3	263-266-9	61832-41-5	61832415	3355	Reach_2851	3667							-6.8	-7.5	-9.2	0.0%	0.0%	0.0%
609-425-1	609-425-1	374067-80-8	374067808	2797	Reach_4301	3668							-6.7	-7.5	-9.2	0.0%	0.0%	0.0%
5-chlorothiophene-2-sulfonyl chloride	700-040-5	674347-28-5	674347285	5985	Reach_4736	3669							-7.7	-7.5	-9.0	0.0%	0.0%	0.0%
Tetrahydro-2-furancarboxylic acid	700-744-2	99842-68-9	99842689	4220	Reach_4984	3670	4.16	0.84	3				-6.6	-7.5	-9.2	0.0%	0.0%	0.0%
11β,16α,17,21-tetrahydroxypregna-1,4-diene-3,20-dione	700-400-1	42831-50-5	42831505	2899	Reach_4887	3671	5.37	0.52	3				-6.8	-7.5	-9.1	0.0%	0.0%	0.0%
2-bromo-7-iodo-9H-fluorene	700-338-5	50372-61-7	50372617	3004	Reach_4867	3672	3.51	1.52	3				-7.7	-7.5	-8.5	0.0%	0.0%	0.0%
3-amino-4-hydroxybenzenesulphonamide	806-756-5	1262985-24-9	1262985249	1804	Reach_5080	3673	1.80	0.50	3				-6.5	-7.5	-9.3	0.0%	0.0%	0.0%
2-bromo-1-(3,5-dihydroxyphenyl)ethanone	620-134-9	1172131-64-4	1172131644	1656	Reach_4559	3674							-6.8	-7.5	-9.2	0.0%	0.0%	0.0%
11β,17,21-trihydroxy-6α-methylpregna-1,4-diene-3,20-dione 21-	220-976-3	2955-88-6	2955886	2569	Reach_1892	3675	4.43	0.91	3				-6.9	-7.5	-9.1	0.0%	0.0%	0.0%
Ethyl 1-(4-methoxyphenyl)-6-(4-nitrophenyl)-7-oxo-4,5,6,7-tetra	611-033-0	536759-91-8	536759918	3108	Reach_4347	3676	3.18	0.18	3				-6.9	-7.5	-9.0	0.0%	0.0%	0.0%
2-pyrrolidin-1-ylethanol	696-003-5	924726-92-1	924726921	4036	Reach_4702	3677	3.99	0.15	3				-7.5	-7.6	-9.2	0.0%	0.0%	0.0%
cis-4-tert-butylcyclohexyl acetate	233-881-7	10411-92-4	10411924	1383	Reach_2290	3678	4.00	0.29	3	3.00	0.29		-7.8	-7.6	-10.1	0.0%	0.0%	0.0%
triisopropyl borate	700-123-6	934985-83-8	934985838	4071	Reach_4770	3679	3.47	0.36	3				-7.8	-7.6	-8.8	0.0%	0.0%	0.0%
ethyl phenylacetate	620-345-6	873055-55-1	873055551	3925	Reach_4567	3680	2.80	0.45	3				-7.8	-7.6	-8.8	0.0%	0.0%	0.0%
3-oxoglutaric acid	210-155-8	608-25-3	608253	3317	Reach_1414	3681	4.22	0.75	3	3.22	0.75		-6.6	-7.6	-9.2	0.0%	0.0%	0.0%
Ethyl 2-(3-formyl-4-hydroxyphenyl)-4-methyl-1,3-thiazole-5-carb	204-320-3	119-40-4	119404	1691	Reach_977	3682	3.89	0.37	3				-7.0	-7.6	-9.1	0.0%	0.0%	0.0%
619-482-4	619-482-4	895525-70-9	895525709	3977	Reach_4522	3683	4.13	1.12	3				-6.8	-7.6	-9.2	0.0%	0.0%	0.0%
labetalol	237-731-1	13951-70-7	13951707	1921	Reach_2353	3684	5.38		2				-6.8	-7.6	-9.1	0.0%	0.0%	0.0%
1,2-dihydro-3H-1,2,4-triazol-3-one	208-835-4	542-92-7	542927	3137	Reach_1348	3685	4.77	0.34	3				-6.7	-7.6	-9.2	0.0%	0.0%	0.0%
620-216-4	620-216-4	298692-41-8	298692418	2575	Reach_4561	3686	3.30		1				-6.7	-7.6	-9.4	0.0%	0.0%	0.0%
benzene-1,2,4,5-tetracarboxylic acid	200-041-6	50-48-6	50486	662	Reach_8	3687	2.89		2				-6.6	-7.6	-9.2	0.0%	0.0%	0.0%
5-amino-3-(4-chlorophenyl)-5-oxopentanoic acid	700-677-9	19190-61-5	19190615	2227	Reach_4965	3688	3.66	0.84	3				-6.8	-7.6	-9.2	0.0%	0.0%	0.0%
4-nitroimidazole	221-224-7	3034-38-6	3034386	2593	Reach_1902	3689	4.27	1.18	3				-6.7	-7.6	-9.3	0.0%	0.0%	0.0%
Ethyl 4-oxocyclohexanecarboxylate	601-635-1	119812-29-2	119812292	5624	Reach_4097	3690							-7.8	-7.6	-9.2	0.0%	0.0%	0.0%
17-hydroxy-19-norpregn-4-ene-3,20-dione 17-acetate	689-732-5	956317-36-5	956317365	4128	Reach_4652	3691	4.91	0.71	3				-7.0	-7.6	-9.0	0.0%	0.0%	0.0%
1H-tetrazol-1-acetic acid	244-551-7	21732-17-2	21732172	2304	Reach_2508	3692	6.40	0.98	3				-6.6	-7.6	-9.3	0.0%	0.0%	0.0%
2-[2-(carboxymethyl)phenoxy]-3,4-dimethylbenzoic acid	941-156-8	1554631-80-9	1554631809	2041	Reach_5180	3693	4.30	0.17	3				-7.0	-7.6	-9.2	0.0%	0.0%	0.0%
4-(2-naphthyl)-1,3-thiazol-2-amine	208-061-7	506-96-7	506967	665	Reach_1314	3694	4.61		1				-7.1	-7.6	-9.1	0.0%	0.0%	0.0%
(1S)-2-(benzylamino)-1-[(2R)-6-fluoro-3,4-dihydro-2H-chromen-2	603-316-2	129050-27-7	129050277	1827	Reach_4116	3695	3.54	0.62	3				-6.8	-7.6	-9.1	0.0%	0.0%	0.0%
3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl acrylate	241-527-8	17527-29-6	17527296	2142	Reach_2436	3696	2.65	1.19	3				-7.8	-7.6	-10.2	0.0%	0.0%	0.0%
retinyl propionate	806-749-7	918504-27-5	918504275	4022	Reach_5079	3697	4.05		2				-7.4	-7.6	-8.4	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
4,4-Difluoro-N-[(1S)-3-hydroxy-1-phenylpropyl]cyclohexanecarb	700-375-7	568572-17-8	568572178	3213	Reach_4880	3698	2.29	0.36	3				-7.0	-7.6	-9.2	0.0%	0.0%	0.0%
N,N'-[Methyl(vinyl)silanediyl]bis(N-ethylacetamide)	608-112-7	27566-05-8	27566058	2512	Reach_4260	3699	3.19	0.27	3				-6.8	-7.6	-9.1	0.0%	0.0%	0.0%
1,2-dibromo-3-chloropropane	700-662-7	950773-38-3	950773383	4119	Reach_4961	3700	1.12	0.33	3				-7.8	-7.6	-9.1	0.0%	0.0%	0.0%
611-200-8	700-160-8	82419-35-0	82419350	3824	Reach_4784	3701							-7.0	-7.6	-9.2	0.0%	0.0%	0.0%
678-409-4	805-125-1	1132940-51-2	1132940512	1616	Reach_5060	3702	2.97	0.12	3				-7.4	-7.6	-8.4	0.0%	0.0%	0.0%
heptadecafluorooctanesulphonyl fluoride	204-200-0	117-61-3	117613	1661	Reach_959	3703	5.30	0.59	3	4.30	0.59		-7.5	-7.6	-9.7	0.0%	0.0%	0.0%
(1R)-2-(benzylamino)-1-[(2S)-6-fluoro-3,4-dihydro-2H-chromen-2	600-381-9	1030385-16-0	1030385160	1356	Reach_4060	3704	3.54	0.62	3				-6.9	-7.6	-9.2	0.0%	0.0%	0.0%
14,14',15,15'-tetradehydro-7,7'-spirobi[dibenzo[b,g][1,9,4,6]diox	695-716-9	1174931-74-8	1174931748	1658	Reach_4694	3705	2.23		1				-7.1	-7.6	-8.7	0.0%	0.0%	0.0%
3-ethyl-4-methyl-1,5-dihydro-2H-pyrrol-2-one	246-857-6	25333-42-0	25333420	2431	Reach_2566	3706	4.49	0.91	3				-7.3	-7.6	-9.2	0.0%	0.0%	0.0%
4-{6-[(methylsulfonyl)oxy]-1-benzothiophen-2-yl}phenyl methan	806-588-2	84449-65-0	84449650	3866	Reach_5076	3707	3.64	0.54	3				-6.9	-7.6	-9.2	0.0%	0.0%	0.0%
5-(methoxymethyl)-2-furaldehyde	700-445-7	846023-54-9	846023549	3870	Reach_4901	3708	3.99		1				-7.8	-7.6	-9.2	0.0%	0.0%	0.0%
5'-chloro-3-hydroxy-2'-methyl-2-naphthanilide	205-207-1	135-63-7	135637	1895	Reach_1134	3709	2.38	0.27	3				-7.0	-7.6	-9.0	0.0%	0.0%	0.0%
diphenhydramine	611-910-8	59886-90-7	59886907	3294	Reach_4368	3710	3.10	1.16	3				-7.1	-7.6	-9.2	0.0%	0.0%	0.0%
4-isothiocyanato-2-(trifluoromethyl)benzonitrile	700-185-4	1122460-01-8	1122460018	1579	Reach_4797	3711	4.26		2				-7.8	-7.6	-8.8	0.0%	0.0%	0.0%
2-amino-3,5-dibromobenzaldehyde	606-376-8	197721-70-3	197721703	2242	Reach_4208	3712	4.20	0.29	3				-7.8	-7.6	-9.2	0.0%	0.0%	0.0%
Dimethyl(octyl)amine oxide	607-854-9	2605-78-9	2605789	2451	Reach_4249	3713	4.83		2				-7.1	-7.6	-9.3	0.0%	0.0%	0.0%
2-(methoxymethyl)benzene-1,4-diamine	679-526-3	337906-36-2	337906362	2686	Reach_4621	3714	3.48	0.20	3	2.48	0.20		-6.9	-7.6	-9.3	0.0%	0.0%	0.0%
Ethyl (2S)-2-[(4S)-4-methyl-2,5-dioxo-1,3-oxazolidin-3-yl]pentanc	616-020-3	7381-13-7	7381137	3627	Reach_4421	3715	4.88	0.33	3	3.88	0.33		-7.1	-7.6	-9.2	0.0%	0.0%	0.0%
methyl 2-{[(4-hydroxyphenyl)sulfonyl]oxy}benzoate	700-604-0	947701-81-7	947701817	4114	Reach_4950	3716	1.76	0.90	3	0.94			-7.0	-7.7	-9.2	0.0%	0.0%	0.0%
ambroxol	609-132-9	35480-52-5	35480525	2739	Reach_4291	3717	3.82	0.35	3				-7.0	-7.7	-9.1	0.0%	0.0%	0.0%
metenolone	700-250-7	849793-87-9	849793879	3882	Reach_4821	3718	4.06	0.61	3				-7.2	-7.7	-9.1	0.0%	0.0%	0.0%
3-[(3-sulfanylbutanoyl)oxy]-2,2-bis{[(3-sulfanylbutanoyl)oxy]met	610-201-0	446292-08-6	446292086	2930	Reach_4327	3719	4.41	0.90	3				-7.0	-7.7	-9.1	0.0%	0.0%	0.0%
(4Z)-hept-4-en-2-yl salicylate	700-488-1	873888-84-7	873888847	3929	Reach_4910	3720	2.58		1				-7.8	-7.7	-9.0	0.0%	0.0%	0.0%
1-Bromomethyl-4-iodo-benzene	618-883-1	92878-95-0	92878950	4052	Reach_4502	3721	3.93		1				-7.9	-7.7	-8.8	0.0%	0.0%	0.0%
3-hydroxy-4-[(2-methyl-5-nitrophenyl)azo]-N-phenylnaphthalen	229-245-3	6448-95-9	6448959	3436	Reach_2188	3722	5.04	1.10	3	4.04	1.10		-7.5	-7.7	-8.3	0.0%	0.0%	0.0%
(phenylethyl)benzene	801-277-8	507448-65-9	507448659	3018	Reach_5055	3723	4.55	0.55	3	3.55	0.55		-7.9	-7.7	-9.0	0.0%	0.0%	0.0%
2-(4-fluorophenyl)thiophene	614-164-1	67911-21-1	67911211	3503	Reach_4396	3724	3.50	2.91	3				-7.9	-7.7	-8.9	0.0%	0.0%	0.0%
(2S)-5-amino-2-[(aminoacetyl)amino]-5-oxopentanoic acid	229-929-1	6843-66-9	6843669	3516	Reach_2207	3725	4.16	0.47	3	3.22	0.60		-6.6	-7.7	-9.4	0.0%	0.0%	0.0%
(4S)-4-cyclohexyl-L-proline	619-510-5	141573-95-7	141573957	1937	Reach_4525	3726	3.17	0.32	3				-6.8	-7.7	-9.3	0.0%	0.0%	0.0%
pentyl 6-deoxy-alpha-L-mannopyranoside	800-300-9	83447-96-5	83447965	3847	Reach_5041	3727	3.63	0.14	3				-6.9	-7.7	-9.3	0.0%	0.0%	0.0%
dimethoxydiphenylsilane	202-662-8	98-37-3	98373	4183	Reach_505	3728	5.68	0.63	3	4.68	0.63		-7.9	-7.7	-9.0	0.0%	0.0%	0.0%
614-164-1	615-149-2	707-36-8	707368	3568	Reach_4411	3729	3.59	0.13	3				-7.9	-7.7	-9.2	0.0%	0.0%	0.0%
2-({[4-(3-methoxypropoxy)-3-methyl-1-oxidopyridin-2-yl]methyl	642-214-2	924663-38-7	924663387	4035	Reach_4609	3730							-6.8	-7.7	-9.4	0.0%	0.0%	0.0%
611-382-9	611-382-9	5637-42-3	5637423	3193	Reach_4358	3731	3.99	0.77	3				-7.1	-7.7	-9.3	0.0%	0.0%	0.0%
cyclohexanecarbonitrile	225-200-7	4711-68-6	4711686	2963	Reach_2058	3732	3.05	0.06	3				-7.9	-7.7	-8.8	0.0%	0.0%	0.0%
3-aminopropane-1-sulphonic acid	222-977-4	3687-18-1	3687181	2780	Reach_1980	3733	5.27	1.08	3				-6.7	-7.7	-9.3	0.0%	0.0%	0.0%
2-(octyloxy)benzoic acid	608-139-4	27830-12-2	27830122	2519	Reach_4262	3734	2.98	0.33	3				-7.2	-7.7	-9.3	0.0%	0.0%	0.0%
17β-hydroxy-1α-methyl-5-αandrostan-3-one acetate	683-287-0	877670-90-1	877670901	3942	Reach_4628	3735	3.63		1				-7.7	-7.7	-9.1	0.0%	0.0%	0.0%
methylidynetri-p-phenylene triisocyanate	687-797-4	23551-91-9	23551919	5786	Reach_4640	3736							-7.3	-7.7	-8.6	0.0%	0.0%	0.0%
1,3-bis[(2-hydroxyethyl)thio]propan-2-ol	230-363-2	7069-42-3	7069423	3567	Reach_2222	3737	5.34	1.68	3	4.34	1.68		-6.8	-7.7	-9.4	0.0%	0.0%	0.0%
16α,17,21-trihydroxypregna-1,4,9(11)-triene-3,20-dione 21-acet	278-593-2	77017-20-0	77017200	3729	Reach_2949	3738	3.91		1				-7.1	-7.7	-9.2	0.0%	0.0%	0.0%
(3S)-3-hydroxy-4,4-dimethyldihydrofuran-2(3H)-one	626-470-2	5405-40-3	5405403	3120	Reach_4580	3739	4.82	1.12	3				-6.9	-7.7	-9.5	0.0%	0.0%	0.0%
5-methylnicotinic acid	608-720-2	3222-49-9	3222499	2645	Reach_4280	3740	5.09	0.69	3				-7.0	-7.7	-9.4	0.0%	0.0%	0.0%
2,6-dimethylphenyl 4-hydroxybenzenesulfonate	700-890-7	503614-91-3	503614913	3002	Reach_5019	3741	4.02		2				-7.1	-7.7	-9.2	0.0%	0.0%	0.0%
methyl 3-aminopyrazinecarboxylate	805-675-2	102340-61-4	102340614	1340	Reach_5069	3742	0.59	0.51	3				-7.1	-7.7	-9.4	0.0%	0.0%	0.0%
methyl 3-amino-5,6-dichloropyrazine-2-carboxylate	600-406-3	103201-78-1	103201781	1360	Reach_4062	3743	3.98	0.75	3				-7.2	-7.7	-9.3	0.0%	0.0%	0.0%
1,3-dihydro-1-oxoisobenzofuran-5-carbonitrile	700-420-0	7605-52-9	7605529	3696	Reach_4895	3744	4.16	0.24	3	3.16	0.24		-7.2	-7.7	-9.4	0.0%	0.0%	0.0%
2,4-dihydro-5-methyl-3H-pyrazol-3-one	203-565-3	108-26-9	108269	1480	Reach_738	3745	1.83	3.09	3				-7.0	-7.7	-9.3	0.0%	0.0%	0.0%
15-tert-butyl 14a-ethyl (2R,6S,12Z,13aS,14aR,16aS)-6-{[(5-methy	700-127-8	21862-63-5	21862635	536	Reach_4771	3746	4.26		2				-7.2	-7.7	-9.3	0.0%	0.0%	0.0%
10-hydroxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl) decan	700-609-8	1231148-36-9	1231148369	1762	Reach_4952	3747	2.48	0.26	3				-7.1	-7.7	-9.1	0.0%	0.0%	0.0%
2-Ethylhexyl-2-cyano-3-(4-methoxyphenyl)-3-phenylprop-2-eno	700-213-5	947753-66-4	947753664	4115	Reach_4806	3748	1.16	0.79	3	0.16	0.79		-7.4	-7.7	-8.7	0.0%	0.0%	0.0%
ethyl (1R,2S)-1-{[(4R)-4-(phenanthridin-6-yloxy)-L-prolyl]amino}-	940-793-9	1432505-97-9	1432505979	1961	Reach_5174	3749	4.57		2				-7.1	-7.7	-9.2	0.0%	0.0%	0.0%
606-247-6	601-489-9	1176-81-4	1176814	1662	Reach_4091	3750	4.16	0.72	3				-7.3	-7.7	-9.4	0.0%	0.0%	0.0%
4,4-Difluoro-N-[(1S)-3-oxo-1-phenylpropyl]cyclohexanecarboxan	700-320-7	18916-17-1	18916171	2215	Reach_4859	3751	5.32		1				-7.2	-7.7	-9.3	0.0%	0.0%	0.0%
627-054-3	627-054-3	82410-32-0	82410320	3823	Reach_4582	3752	5.32	1.60	3				-6.7	-7.7	-9.4	0.0%	0.0%	0.0%
Methyl 5-amino-4-cyano-3-methylthiophene-2-carboxylate	700-422-1	61320-65-8	61320658	3331	Reach_4896	3753	4.04		2				-7.2	-7.7	-9.4	0.0%	0.0%	0.0%
616-651-4	700-301-3	69739-16-8	69739168	3549	Reach_4851	3754	4.14	0.91	3				-7.7	-7.8	-8.3	0.0%	0.0%	0.0%
2-[3-hydroxy-4-(phenylcarbonyl)phenoxy]ethyl 2-methylprop-2-(	700-105-8	16613-04-0	16613040	2102	Reach_4765	3755	3.53	0.26	3				-7.2	-7.8	-9.2	0.0%	0.0%	0.0%
3-amino-4-chlorobenzamide	243-231-4	19694-10-1	19694101	2236	Reach_2482	3756	5.08		1				-7.0	-7.8	-9.4	0.0%	0.0%	0.0%
604-269-0	303-725-3	94213-23-7	94213237	4099	Reach_3009	3757	3.00	0.70	3				-7.9	-7.8	-9.2	0.0%	0.0%	0.0%
tetraammonium ethylenediaminetetraacetate	245-022-3	22473-78-5	22473785	1206	Reach_2523	3758	5.10	0.71	4	4.53	0.98		-7.5	-7.8	-9.1	0.0%	0.0%	0.0%
610-915-2	630-348-4	84268-36-0	84268360	3858	Reach_4598	3759	3.32	0.30	3				-8.0	-7.8	-9.2	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
2-[4-(Phenylmethoxy)phenyl]ethyldecanoate	700-058-3	848484-93-5	848484935	3877	Reach_4744	3760	1.69	0.50	3				-7.4	-7.8	-8.4	0.0%	0.0%	0.0%
pent-4-enoyl chloride	444-370-5	669005-94-1	669005941	3483	Reach_3737	3761	1.06	2.30	3				-8.0	-7.8	-9.4	0.0%	0.0%	0.0%
601-596-0	700-336-4	1141-23-7	1141237	1624	Reach_4866	3762	4.57	1.30	3				-7.1	-7.8	-9.3	0.0%	0.0%	0.0%
2-(methylsulfonyl)-3-nitropyrazolo[1,5-a]pyridine	223-768-0	4062-46-8	4062468	2861	Reach_2008	3763	3.00		1				-7.0	-7.8	-9.5	0.0%	0.0%	0.0%
4'-chloro-3-hydroxy-2',5'-dimethoxy-2-naphthanilide	224-270-6	4273-92-1	4273921	2898	Reach_2025	3764	2.84	0.25	3				-7.1	-7.8	-9.2	0.0%	0.0%	0.0%
(2R)-6-fluoro-2-[(2S)-oxiran-2-yl]chromane	603-315-7	129050-26-6	129050266	1826	Reach_4115	3765	3.73	1.25	3				-8.0	-7.8	-9.3	0.0%	0.0%	0.0%
(6-hydroxy-2-naphthyl)boronic acid	687-349-8	173194-95-1	173194951	2131	Reach_4633	3766							-7.0	-7.8	-9.4	0.0%	0.0%	0.0%
(17β)-17-hydroxyestra-4,6-dien-3-one	268-028-8	67990-05-0	67990050	3504	Reach_2895	3767	5.04	1.10	3	4.04	1.10		-7.2	-7.8	-9.3	0.0%	0.0%	0.0%
617-838-3	606-946-6	221640-14-8	221640148	5780	Reach_4228	3768	4.00		2				-6.8	-7.8	-9.5	0.0%	0.0%	0.0%
619-739-0	700-318-6	879671-67-7	879671677	6073	Reach_4858	3769							-8.0	-7.8	-9.2	0.0%	0.0%	0.0%
benzyl (5-{[4-({5-[acetyl(hydroxy)amino]pentyl}amino)-4-oxobut	218-378-2	2137-18-0	2137180	2292	Reach_1762	3770	2.60		1				-6.9	-7.8	-9.5	0.0%	0.0%	0.0%
(1E)-1-chloro-3,3,3-trifluoroprop-1-ene	700-486-0	102687-65-0	102687650	1351	Reach_4909	3771	5.02	0.50	3	4.02	0.50		-8.1	-7.8	-10.1	0.0%	0.0%	0.0%
603-467-4	603-467-4	13127-18-9	13127189	1848	Reach_4122	3772	5.10	0.70	3	4.10	0.70		-7.9	-7.8	-9.4	0.0%	0.0%	0.0%
2-[2-(dimethylamino)ethyl]-2,3-dihydro-1H-inden-1-one	700-600-9	3409-21-0	3409210	2691	Reach_4947	3773	3.72	0.70	3				-7.5	-7.8	-9.4	0.0%	0.0%	0.0%
(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl methanesulfonate	700-367-3	35130-97-3	35130973	2724	Reach_4876	3774	4.87	1.01	3				-7.1	-7.8	-9.5	0.0%	0.0%	0.0%
(2R)-6-fluoro-2-[(2R)-oxiran-2-yl]chromane	606-373-1	197706-50-6	197706506	2240	Reach_4206	3775	3.73	1.25	3				-8.0	-7.8	-9.3	0.0%	0.0%	0.0%
(2S)-6-fluoro-2-[(2S)-oxiran-2-yl]chromane	603-314-1	129050-23-3	129050233	1825	Reach_4114	3776	3.73	1.25	3				-8.0	-7.8	-9.3	0.0%	0.0%	0.0%
(1S)-2,3,4,6-tetra-O-acetyl-1,5-anhydro-1-[4-chloro-3-(4-ethoxyb	930-010-9	461432-25-7	461432257	2947	Reach_5129	3777	3.36	0.46	3				-7.2	-7.8	-9.3	0.0%	0.0%	0.0%
(1S)-3-(methylamino)-1-(2-thienyl)propan-1-ol	696-192-4	935859-71-5	935859715	4074	Reach_4709	3778	3.99	0.18	3				-7.1	-7.8	-9.5	0.0%	0.0%	0.0%
(2R)-2,8-dimethyl-2-[(4R,8R)-4,8,12-trimethyltridecyl]-3,4-dihydr	606-247-6	191605-10-4	191605104	2223	Reach_4200	3779	4.45	0.81	3				-7.7	-7.8	-8.3	0.0%	0.0%	0.0%
6-Chlorohexanoic acid	212-406-7	814-80-2	814802	6042	Reach_1551	3780	5.75	0.50	3	5.14	0.48		-7.4	-7.8	-9.5	0.0%	0.0%	0.0%
2-tert-butyl-4,6-diiodophenol	805-179-6	60803-26-1	60803261	3316	Reach_5063	3781	3.04	0.31	3				-7.9	-7.8	-9.3	0.0%	0.0%	0.0%
2-[(3-nitropyrazolo[1,5-a]pyridin-2-yl)oxy]ethanol	689-267-8	501925-98-0	501925980	2997	Reach_4650	3782	4.20	0.21	3				-7.0	-7.8	-9.5	0.0%	0.0%	0.0%
N-[(2-methyl-5-nitrophenyl)carbamothioyl]acetamide	607-485-3	25015-63-8	25015638	2413	Reach_4242	3783	5.79	0.77	3	4.79	0.77		-7.0	-7.9	-9.7	0.0%	0.0%	0.0%
2-(2-Methoxyphenoxy)ethanamine	700-396-1	60924-38-1	60924381	3320	Reach_4886	3784	4.14	0.70	3				-7.6	-7.9	-9.5	0.0%	0.0%	0.0%
1,4,5,6-tetrahydro-1,2-dimethylpyrimidine	260-375-3	56773-42-3	56773423	5936	Reach_2822	3785	4.68	0.43	3	3.93	0.56		-8.1	-7.9	-9.2	0.0%	0.0%	0.0%
4-({4-[4-(4-{[4-(Propan-2-yloxy)phenyl]sulfonyl}phenoxy)butoxy]	638-778-4	376348-77-5	376348775	2803	Reach_4602	3786	3.74	0.88	3				-7.3	-7.9	-8.8	0.0%	0.0%	0.0%
601-489-9	619-702-9	33494-80-3	33494803	5848	Reach_4538	3787							-7.2	-7.9	-9.4	0.0%	0.0%	0.0%
605-935-3	605-935-3	181525-38-2	181525382	2168	Reach_4184	3788							-7.0	-7.9	-9.4	0.0%	0.0%	0.0%
(2S)-6-fluoro-2-[(2R)-oxiran-2-yl]chromane	606-374-7	197706-51-7	197706517	2241	Reach_4207	3789	3.73	1.25	3				-8.1	-7.9	-9.4	0.0%	0.0%	0.0%
(2S)-pentan-2-ol	680-808-3	106261-64-7	106261647	5598	Reach_4627	3790							-8.1	-7.9	-9.0	0.0%	0.0%	0.0%
strontium 4-[(4-chloro-5-methyl-2-sulphonatophenyl)azo]-3-hyd	267-291-6	67828-72-2	67828722	5988	Reach_2890	3791	5.28		1				-7.6	-7.9	-9.2	0.0%	0.0%	0.0%
(5R)-5-[(1S)-1,2-Dihydroxyethyl]-4-ethoxy-3-hydroxyfuran-2(5H)	617-849-3	86404-04-8	86404048	3906	Reach_4477	3792	4.75	0.90	3				-7.0	-7.9	-9.7	0.0%	0.0%	0.0%
phenethylamine	700-928-2	143782-23-4	143782234	1970	Reach_5028	3793	2.61	0.44	3				-8.1	-7.9	-9.0	0.0%	0.0%	0.0%
(3aS,4R,5S,6S,8R,9R,9aR,10R)-6-ethenyl-5-hydroxy-4,6,9,10-tetra	700-114-7	143183-03-3	143183033	1958	Reach_4768	3794	0.21	1.16	3				-7.2	-7.9	-9.5	0.0%	0.0%	0.0%
chloromethyl chlorosulphate	700-938-7	72716-26-8	72716268	6012	Reach_5031	3795	4.50		2				-8.1	-7.9	-9.5	0.0%	0.0%	0.0%
1-tert-butyl-3,5-diiodo-2-methoxybenzene	229-102-5	6410-32-8	6410328	3424	Reach_2178	3796	5.04	1.10	3	4.04	1.10		-8.0	-7.9	-9.0	0.0%	0.0%	0.0%
hexane-1,6-diyl bis{[3-(trimethoxysilyl)propyl]carbamate}	610-764-2	51997-51-4	51997514	3050	Reach_4335	3797	3.72	0.33	3				-7.2	-7.9	-9.6	0.0%	0.0%	0.0%
undec-10-en-1-yl 2-cyano-3,3-diphenylacrylate	806-439-1	1364731-90-7	1364731907	1900	Reach_5072	3798	3.73	0.27	3	2.73	0.27		-7.5	-7.9	-8.5	0.0%	0.0%	0.0%
bis(nonafluorobutyl)phosphinic acid	248-660-0	27794-93-0	27794930	5812	Reach_2612	3799	5.41		2	4.48			-8.3	-7.9	-9.6	0.0%	0.0%	0.0%
700-627-6	610-150-4	438193-30-7	438193307	5887	Reach_4324	3800	3.18		1				-8.0	-7.9	-8.8	0.0%	0.0%	0.0%
2-(octyloxy)benzoyl chloride	250-799-7	31775-20-9	31775209	2632	Reach_2656	3801	5.26	1.21	3	4.26	1.21		-8.1	-7.9	-9.2	0.0%	0.0%	0.0%
Propane-1,3-diyl dioctanoate	700-787-7	769953-18-6	769953186	6034	Reach_4994	3802	5.46	0.23	3	4.46	0.23		-8.0	-7.9	-9.1	0.0%	0.0%	0.0%
Tripropan-2-ylsilyl 2-methylprop-2-enoate	700-182-8	134652-60-1	134652601	1880	Reach_4795	3803							-8.1	-7.9	-10.6	0.0%	0.0%	0.0%
trans-4-tert-butylcyclohexanol	202-667-5	98-42-0	98420	4184	Reach_506	3804	5.34		2				-8.2	-7.9	-9.0	0.0%	0.0%	0.0%
2,2-dimethoxy-1,2-diphenylethan-1-one	680-046-1	74462-02-5	74462025	3637	Reach_4623	3805	2.36		2				-8.0	-7.9	-9.5	0.0%	0.0%	0.0%
7,7,8,9,9-pentamethyl-6,7,8,9-tetrahydro-5H-cyclopenta[h]quina	801-093-8	1315251-11-6	1315251116	1849	Reach_5052	3806	2.67	0.29	3	1.67	0.29		-7.6	-7.9	-9.2	0.0%	0.0%	0.0%
4-(Oxiran-2-ylmethoxy)-9H-carbazole	601-680-7	120202-68-8	120202688	5625	Reach_4100	3807							-7.6	-7.9	-9.6	0.0%	0.0%	0.0%
Tert-butyl 3-oxoazetidine-1-carboxylate	605-390-1	165115-73-1	165115731	2095	Reach_4173	3808	3.87	1.16	3				-7.4	-8.0	-9.5	0.0%	0.0%	0.0%
(chloromethyl)(methoxy)dimethylsilane	300-199-7	93924-07-3	93924073	4092	Reach_3004	3809	1.82	0.10	3				-8.2	-8.0	-9.7	0.0%	0.0%	0.0%
617-556-0	609-734-1	39648-67-4	39648674	2845	Reach_4310	3810	2.96	0.34	3				-7.1	-8.0	-9.6	0.0%	0.0%	0.0%
2-({1-[(2-methoxyphenyl)amino]-1,3-dioxobutan-2-yl}diazenyl)be	691-722-0	154477-55-1	154477551	2036	Reach_4670	3811	2.11		2				-7.2	-8.0	-9.5	0.0%	0.0%	0.0%
5-bromonicotinic acid	244-065-5	20826-04-4	20826044	2275	Reach_2500	3812	3.26	1.17	3				-7.3	-8.0	-9.6	0.0%	0.0%	0.0%
2-chloro-1,1,1-triethoxyethane	628-654-8	51076-95-0	51076950	3027	Reach_4587	3813	3.95	0.71	3				-8.2	-8.0	-9.1	0.0%	0.0%	0.0%
(1R,2S,5R)-5-methyl-2-(propan-2-yl)cyclohexyl (ethylamino)(oxo	209-502-6	583-39-1	583391	3244	Reach_1382	3814	3.85	0.80	3	2.85	0.80		-7.7	-8.0	-9.5	0.0%	0.0%	0.0%
(2R)-2-methyloxirane	800-036-4	1422423-64-0	1422423640	5694	Reach_5035	3815	4.82		1				-8.3	-8.0	-9.6	0.0%	0.0%	0.0%
4-[(4-oxo-1,4-dihydropyrimidin-2- yl)amino]benzonitrile	606-195-4	189956-45-4	189956454	2220	Reach_4197	3816							-7.2	-8.0	-9.5	0.0%	0.0%	0.0%
hexanoic anhydride	687-786-4	1246610-75-2	1246610752	5638	Reach_4638	3817							-8.2	-8.0	-9.7	0.0%	0.0%	0.0%
phentermine	200-991-1	76-89-1	76891	3726	Reach_178	3818	1.80	3.22	3				-8.2	-8.0	-9.8	0.0%	0.0%	0.0%
2-(Diethylamino)ethyl 4-{[2-(octyloxy)benzoyl]amino}benzoate	692-852-0	26090-29-9	26090299	2453	Reach_4681	3819	1.76	0.28	3				-7.6	-8.0	-8.9	0.0%	0.0%	0.0%
695-716-9	629-247-8	183208-35-7	183208357	2180	Reach_4590	3820	4.05		2				-7.6	-8.0	-8.7	0.0%	0.0%	0.0%
2-(methylthio)-3-nitropyrazolo[1,5-a]pyridine	619-167-1	95748-46-2	95748462	4132	Reach_4511	3821	4.47	1.05	3				-7.7	-8.0	-9.6	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
5,7-di-tert-butyl-3-[4-(2-hydroxyethoxy)phenyl]-1-benzofuran-2(	940-050-9	1216942-04-9	1216942049	1734	Reach_5164	3822	2.17	0.16	3				-7.4	-8.0	-9.3	0.0%	0.0%	0.0%
2-chloro-6,7-dimethoxyquinazolin-4-amine	245-821-7	23680-84-4	23680844	2354	Reach_2532	3823	3.78	0.75	3				-7.3	-8.0	-9.6	0.0%	0.0%	0.0%
2-[2-(2,4-difluorophenyl)prop-2-en-1-yl]propane-1,3-diol	690-742-7	1266664-66-7	1266664667	5645	Reach_4661	3824	3.68		2				-7.5	-8.0	-9.6	0.0%	0.0%	0.0%
5-tert-butyl-3-methyl-1,2-phenylene dibenzoate	691-553-2	1232839-86-9	1232839869	1766	Reach_4669	3825	1.46	1.27	3				-7.6	-8.0	-8.9	0.0%	0.0%	0.0%
9β,11β-epoxy-17,21-dihydroxy-16α-methylpregna-1,4-diene-3,2	246-529-2	24916-90-3	24916903	2406	Reach_2556	3826	4.95	0.26	3				-7.3	-8.0	-9.5	0.0%	0.0%	0.0%
retinol	200-683-7	68-26-8	68268	3514	Reach_93	3827	4.89	1.33	3	3.89	1.33		-7.7	-8.0	-9.0	0.0%	0.0%	0.0%
629-671-3	213-214-6	930-33-6	930336	4057	Reach_1606	3828	5.76	0.86	3				-8.2	-8.0	-9.4	0.0%	0.0%	0.0%
4-butylbenzene-1,3-diol	700-906-2	22450-96-0	22450960	5783	Reach_5022	3829	4.45		1				-7.9	-8.0	-9.6	0.0%	0.0%	0.0%
pyridine-2,4-dicarboxylic acid	207-892-2	499-80-9	499809	2991	Reach_1298	3830							-7.3	-8.0	-9.7	0.0%	0.0%	0.0%
methyl trichloroacetate	209-960-7	598-99-2	598992	3295	Reach_1407	3831	4.61	1.54	3				-8.3	-8.0	-9.5	0.0%	0.0%	0.0%
N-Palmitoylglycine	627-023-4	2441-41-0	2441410	2392	Reach_4581	3832	2.06	0.31	3				-7.5	-8.0	-9.6	0.0%	0.0%	0.0%
9-fluoro-11β,17,21-trihydroxy-16β-methylpregna-1,4-diene-3,20	609-203-4	36130-02-6	36130026	2757	Reach_4292	3833	3.75	0.11	3				-7.4	-8.0	-9.5	0.0%	0.0%	0.0%
(2Z,16Z)-4,15-dioxo-5,8,11,14-tetraoxaoctadeca-2,16-diene-1,18	806-734-5	109828-01-5	109828015	1509	Reach_5078	3834	5.01		1				-7.1	-8.0	-9.7	0.0%	0.0%	0.0%
4-[(2,4-dichloro-5-methoxyphenyl)amino]-6-methoxy-7-[3-(4-me	601-437-5	116539-55-0	116539550	1651	Reach_4089	3835	4.29	0.84	3	3.29	0.84		-7.4	-8.0	-9.5	0.0%	0.0%	0.0%
1,1,1-Trimethoxy-2-methylpropane	606-318-1	19478-81-0	19478810	5760	Reach_4204	3836							-8.3	-8.0	-9.6	0.0%	0.0%	0.0%
4,4-dimethyl-1,2-oxazolidin-3-one	629-718-8	127946-77-4	127946774	5651	Reach_4595	3837	4.90		2				-7.7	-8.1	-9.7	0.0%	0.0%	0.0%
6-hydroxy-3,4-dihydroquinolin-2(1H)-one	700-003-3	56519-71-2	56519712	3200	Reach_4721	3838	5.05	0.44	3	4.05	0.44		-7.3	-8.1	-9.6	0.0%	0.0%	0.0%
ethyl 2-cyano-3-oxobutanoate	602-769-3	122397-96-0	122397960	1749	Reach_4104	3839	3.11		1				-8.2	-8.1	-9.7	0.0%	0.0%	0.0%
Octadecyl 2-[(E)-(5-cyano-1-dodecyl-2-hydroxy-4-methyl-6-oxo-1	610-309-8	4651-94-9	4651949	2955	Reach_4328	3840	3.74	0.58	3				-7.4	-8.1	-9.6	0.0%	0.0%	0.0%
608-783-6	695-996-2	510729-01-8	510729018	3026	Reach_4701	3841	3.45	0.44	3				-8.3	-8.1	-9.9	0.0%	0.0%	0.0%
1-bromooctane	203-912-9	111-83-1	111831	312	Reach_874	3842	2.92		1				-8.3	-8.1	-10.3	0.0%	0.0%	0.0%
propiolactone	200-340-1	57-57-8	57578	3233	Reach_42	3843	4.54	1.02	3				-8.2	-8.1	-9.7	0.0%	0.0%	0.0%
1-Chloro-3,5-dimethyladamantane	616-314-1	76272-34-9	76272349	3707	Reach_4433	3844	3.80	0.70	3				-8.3	-8.1	-10.1	0.0%	0.0%	0.0%
16-{{(1S)-1-carboxy-4-[(2,5-dioxopyrrolidin-1-yl)oxy]-4-oxobutyl}	700-853-5	943586-12-7	943586127	4102	Reach_5013	3845	3.42	1.24	3				-7.4	-8.1	-9.8	0.0%	0.0%	0.0%
1H-indazole-3-carboxylic acid	601-596-0	119302-24-8	119302248	1688	Reach_4095	3846	2.64		2				-7.3	-8.1	-9.7	0.0%	0.0%	0.0%
3-Methoxy-3-methylbutyl acetate	700-029-5	824-80-6	824806	6044	Reach_4450	3847							-8.3	-8.1	-9.3	0.0%	0.0%	0.0%
Ethyl 3-(difluoromethyl)-1-methyl-1H-pyrazole-4-carboxylate	804-748-6	1216941-97-7	1216941977	1732	Reach_5057	3848	3.82	0.92	3				-7.4	-8.1	-9.7	0.0%	0.0%	0.0%
Alkanes, C10-14	220-254-8	2688-84-8	2688848	2490	Reach_1854	3849	3.74	0.53	3				-8.3	-8.1	-10.4	0.0%	0.0%	0.0%
vinylene carbonate	212-825-5	872-36-6	872366	3923	Reach_1579	3850	3.65	0.21	3	2.65	0.21		-7.7	-8.1	-9.9	0.0%	0.0%	0.0%
2-methylquinolin-8-amine	606-190-7	18978-78-4	18978784	2218	Reach_4195	3851	3.82	0.60	3				-7.7	-8.1	-9.7	0.0%	0.0%	0.0%
1,5,2,4-dioxadithiane 2,2,4,4-tetraoxide	700-464-0	99591-74-9	99591749	4207	Reach_4903	3852	4.70	0.11	3	3.70	0.11		-7.3	-8.1	-9.8	0.0%	0.0%	0.0%
1,1,1,3,4,4,4-heptafluoro-3-(trifluoromethyl)butan-2-one	690-995-3	756-12-7	756127	3677	Reach_4663	3853	4.70		2				-8.4	-8.1	-10.6	0.0%	0.0%	0.0%
2-methylresorcinol	213-313-4	936-49-2	936492	4076	Reach_1611	3854	4.09	0.81	3	3.11	1.32		-7.5	-8.1	-9.7	0.0%	0.0%	0.0%
2-chloro-5-nitrobenzoic acid	219-739-7	2516-96-3	2516963	2421	Reach_1826	3855	4.18	0.46	3				-7.5	-8.2	-9.9	0.0%	0.0%	0.0%
4,4'-(2-ethylhexane-1,1-diyl)diphenol	246-386-6	24650-42-8	24650428	2400	Reach_2552	3856	4.34	0.11	3	3.34	0.11		-7.9	-8.2	-9.5	0.0%	0.0%	0.0%
611-909-2	241-543-5	17572-97-3	17572973	5740	Reach_2437	3857	4.62		2				-7.4	-8.2	-9.8	0.0%	0.0%	0.0%
cyclopentadiene	692-842-6	1312296-85-7	1312296857	5660	Reach_4680	3858	5.19		1				-8.5	-8.2	-10.5	0.0%	0.0%	0.0%
4,4,5,5-Tetramethyl-1,3,2-dioxaborolane	691-441-3	1316184-79-8	1316184798	5662	Reach_4667	3859							-8.4	-8.2	-9.4	0.0%	0.0%	0.0%
deferoxamine	200-738-5	70-51-9	70519	3564	Reach_96	3860	5.72	2.44	3				-7.3	-8.2	-10.0	0.0%	0.0%	0.0%
(2S)-tetrahydrofuran-2-carboxylic acid	677-278-0	89402-42-6	89402426	3974	Reach_4617	3861	2.54	0.29	3				-7.3	-8.2	-9.9	0.0%	0.0%	0.0%
2-(3,5-dimethylhex-3-en-2-yloxy)-2-methylpropyl cyclopropanec	700-118-9	676532-44-8	676532448	3498	Reach_4769	3862	3.76		1				-8.4	-8.2	-9.7	0.0%	0.0%	0.0%
methyl 2-methyl-2-phenylpropanoate	617-556-0	84348-37-8	84348378	3861	Reach_4467	3863	4.95	1.20	3				-8.5	-8.2	-9.4	0.0%	0.0%	0.0%
(2S)-2-{[(5-methylpyrazin-2-yl)carbonyl]amino}non-8-enoic acid	700-643-3	155794-06-2	155794062	2044	Reach_4958	3864	2.47	0.23	3				-7.6	-8.2	-9.7	0.0%	0.0%	0.0%
methyl cis-3-methylcyclohexanecarboxylate	680-002-1	145022-44-2	145022442	5699	Reach_4622	3865	5.03		2				-8.5	-8.3	-9.6	0.0%	0.0%	0.0%
1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluorooctane	688-332-8	199119-58-9	199119589	5764	Reach_4644	3866	2.31	2.46	3	2.04	2.47		-8.5	-8.3	-10.7	0.0%	0.0%	0.0%
Octan-2-yl 2-cyanoacrylate	938-829-3	936103-10-5	936103105	4075	Reach_5154	3867	4.15	0.39	3				-8.5	-8.3	-9.7	0.0%	0.0%	0.0%
(Bromomethyl)cyclobutane	261-858-1	59690-88-9	59690889	5943	Reach_2840	3868	6.46		2				-8.6	-8.3	-10.4	0.0%	0.0%	0.0%
Ethyl [(5-chlorothiophen-2-yl)sulfonyl]carbamate	700-455-1	380843-75-4	380843754	2814	Reach_4902	3869	2.38	0.40	3				-7.7	-8.4	-10.0	0.0%	0.0%	0.0%
O,S-dibutyl dithioimidodicarbonate	691-061-8	1001320-38-2	1001320382	1294	Reach_4664	3870	2.77		2				-8.6	-8.4	-9.9	0.0%	0.0%	0.0%
methyl 2-[4-(4-{4-[hydroxy(diphenyl)methyl]piperidin-1-yl}butan	601-595-5	119302-20-4	119302204	1687	Reach_4094	3871	3.72	0.62	3				-7.9	-8.4	-9.5	0.0%	0.0%	0.0%
689-732-5	611-173-2	54605-02-6	54605026	3148	Reach_4350	3872	3.45	0.23	3				-7.8	-8.4	-10.0	0.0%	0.0%	0.0%
3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl 2-chloroacrylate	801-260-5	96383-55-0	96383550	4146	Reach_5054	3873	2.56	0.96	3				-8.6	-8.5	-11.1	0.0%	0.0%	0.0%
609-203-4	627-725-0	398489-26-4	398489264	2850	Reach_4585	3874	3.93	1.08	3				-7.8	-8.5	-10.0	0.0%	0.0%	0.0%
800-300-9	692-895-5	81778-07-6	81778076	3813	Reach_4682	3875	4.48	1.41	3				-8.7	-8.5	-9.8	0.0%	0.0%	0.0%
(2Z)-1,1,1,4,4,4-Hexafluorobut-2-ene	700-651-7	692-49-9	692499	3536	Reach_4960	3876	4.52	0.28	3	3.52	0.28		-8.7	-8.5	-10.9	0.0%	0.0%	0.0%
611-173-2	606-191-2	18979-61-8	18979618	2219	Reach_4196	3877	3.77		2				-7.8	-8.5	-10.0	0.0%	0.0%	0.0%
bromoethylene	606-080-9	18637-00-8	18637008	5749	Reach_4192	3878	4.47		1				-8.9	-8.5	-10.8	0.0%	0.0%	0.0%
2-({[3-(methylthio)phenyl]carbamoyl}oxy)ethyl acrylate	700-694-1	1207339-61-4	1207339614	1719	Reach_4970	3879	3.00		1				-8.7	-8.6	-10.1	0.0%	0.0%	0.0%
acetyl bromide	606-740-6	21331-43-1	21331431	2290	Reach_4216	3880	3.05		2				-8.8	-8.6	-10.4	0.0%	0.0%	0.0%
2-methyl-2-(1-methylpropyl)propane-1,3-diol	212-387-5	813-60-5	813605	3805	Reach_1550	3881	4.81	1.23	3				-8.8	-8.6	-10.2	0.0%	0.0%	0.0%
methyl cyclohexylacetate	805-128-8	54981-42-9	54981429	5928	Reach_5062	3882							-8.9	-8.7	-9.9	0.0%	0.0%	0.0%
2,3-difluoro-5-(trifluoromethyl)pyridine	627-872-0	1514-82-5	1514825	2019	Reach_4586	3883	4.33	0.99	3	3.33	0.99		-9.0	-8.7	-10.7	0.0%	0.0%	0.0%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]		TP(Cwcoast) [-]
607-821-9	607-821-9	25858-24-6	25858246	2445	Reach_4248	3884	2.38	0.72	3				-8.1	-8.7	-10.1	0.0%	0.0%		0.0%
2,3,3,3-tetrafluoro-2-(trifluoromethyl)propanenitrile	806-451-7	42532-60-5	42532605	2895	Reach_5073	3885							-8.9	-8.7	-11.0	0.0%	0.0%		0.0%
(1R,2S,5R)-5-methyl-2-(propan-2-yl)-N-[2-(pyridin-2-yl)ethyl]cycl	700-097-6	847565-09-7	847565097	3876	Reach_4760	3886	4.49		2				-8.1	-8.7	-10.2	0.0%	0.0%		0.0%
2-bromo-3,3,3-trifluoroprop-1-ene	618-003-6	87392-07-2	87392072	3930	Reach_4484	3887	5.70	0.59	3				-9.0	-8.7	-11.0	0.0%	0.0%		0.0%
Methyl 2,2,3,3,4,4-hexafluoro-4-[(trifluorovinyl)oxy]butanoate	700-713-3	83161-22-2	83161222	3841	Reach_4976	3888	6.00	0.91	3				-9.0	-8.8	-11.4	0.0%	0.0%		0.0%
2,5-Bis-O-{4-[4-(acryloyloxy)benzoyl]-3-methoxybenzoyl}-1,4:3,6	700-376-2	1015689-48-1	1015689481	1324	Reach_4881	3889	2.17	1.09	3				-8.2	-8.9	-10.4	0.0%	0.0%		0.0%
Methyl butylcarbamate	805-660-0	2594-21-0	2594210	2447	Reach_5068	3890	3.41	1.31	3				-9.1	-8.9	-10.3	0.0%	0.0%		0.0%
2,2,3,3-Tetrafluorooxetane	700-202-5	765-63-9	765639	3718	Reach_4801	3891	3.63		2				-9.4	-9.1	-11.3	0.0%	0.0%		0.0%
ethyl cyclopent-2-en-1-ylacetate	605-150-6	15848-49-4	15848494	2062	Reach_4168	3892	4.29	0.31	3	3.39	0.39		-9.5	-9.3	-10.7	0.0%	0.0%		0.0%
3-[(4R)-4-Isopropylcyclohex-1-en-1-yl]propanal	700-886-5	1378867-81-2	1378867812	1914	Reach_5018	3893	3.34		2				-9.7	-9.4	-10.6	0.0%	0.0%		0.0%
3-(cyclohexyloxy)propane-1,2-diol	805-622-3	10305-41-6	10305416	1358	Reach_5067	3894	5.66	0.97	3				-9.5	-10.1	-11.6	0.0%	0.0%		0.0%
octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	218-216-0	2082-79-3	2082793	2276	Reach_1755	3895	-1.89	1.02	3	3.30									
2,6,10,15,19,23-hexamethyltetracosane	203-825-6	111-01-3	111013	1535	Reach_841	3896	-3.17	1.15	3										
1,3,5-tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6(	248-597-9	27676-62-6	27676626	2516	Reach_2611	3897	-1.26	3.01	3	5.00									
5,5'-(1H-isoindole-1,3(2H)-diylidene)dibarbituric acid	253-256-2	36888-99-0	36888990	2783	Reach_2706	3898	7.04		1										
607-578-9	203-727-3	110-00-9	110009	270	Reach_799	3899	4.80		2										
docos-1-ene	222-023-7	3320-83-0	3320830	2677	Reach_1946	3900	3.73	0.88	3	2.73	0.88								
692-514-2	248-503-6	27511-79-1	27511791	5810	Reach_2609	3901													
2,6,10,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaene	203-826-1	111-02-4	111024	1536	Reach_842	3902	-1.72	0.90	3										
(Z)-N-octadecyldocos-13-enamide	233-226-5	10094-45-8	10094458	1313	Reach_2281	3903	-3.58	2.70	3										
O,O'-dioctadecylpentaerythritol bis(phosphite)	223-276-6	3806-34-6	3806346	2813	Reach_1993	3904	-3.88	1.31	3										
4,4'-bis[4-[bis(2-hydroxyethyl)amino]-6-anilino-1,3,5-triazin-2-yl]	224-548-7	4404-43-7	4404437	641	Reach_2033	3905	5.03	0.82	3	4.40	0.63								
N,N'-(2-chloro-1,4-phenylene)bis[4-[(2,5-dichlorophenyl)azo]-3-h	226-106-9	5280-78-4	5280784	3075	Reach_2091	3906	-1.05	3.55	3	4.00									
tetracosanol	208-043-9	506-51-4	506514	3014	Reach_1311	3907	-1.06	0.99	3										
(Z)-octadec-9-enyl oleate	222-980-0	3687-45-4	3687454	2781	Reach_1981	3908	-3.49	3.06	3										
2,2-bis[[(1-oxoisononyl)oxy]methyl]-1,3-propanediyl diisononana	298-364-0	93803-89-5	93803895	4083	Reach_2997	3909	-1.86	2.32	3										
dihexadecyl peroxodicarbonate	247-611-0	26322-14-5	26322145	2464	Reach_2579	3910	-3.34	2.23	3										
hexadecyl 3,5-bis-tert-butyl-4-hydroxybenzoate	267-342-2	67845-93-6	67845936	3501	Reach_2891	3911	-1.03	0.70	3										
ditetradecyl peroxydicarbonate	258-436-4	53220-22-7	53220227	3092	Reach_2790	3912	-2.05	1.78	3										
N,N'-phenylene-1,4-bis[4-[(2,5-dichlorophenyl)azo]-3-hydroxyna	225-730-9	5036-48-6	5036486	3003	Reach_2072	3913	5.22	0.65	3	4.22	0.65								
N,N'-(2,5-dichloro-1,4-phenylene)bis[4-[(2,5-dichlorophenyl)azo]	255-005-2	40618-31-3	40618313	2860	Reach_2732	3914	-1.36	3.78	3	4.00									
(Z)-N-octadec-9-enylhexadecan-1-amide	240-367-6	16260-09-6	16260096	2086	Reach_2416	3915	-2.09	1.94	3										
(1S)-1,5-anhydro-2,3,4,6-tetrakis-O-(2,2-dimethylpropanoyl)-1-(3	695-878-0	1283129-18-9	1283129189	1819	Reach_4696	3916	-1.03	1.35	3										
618-295-5	618-295-5	897626-46-9	897626469	3984	Reach_4490	3917	-6.24	4.49	3	1.80									
glycerol tristearate	209-097-6	555-43-1	555431	3174	Reach_1365	3918	-6.25	4.21	3	5.00									
1-amino-4-(3-amino-2,4,6-trimethyl-5-sulphoanilino)-9,10-dihyd	246-025-2	24124-40-1	24124401	2374	Reach_2539	3919	5.08		1										
N,N'-(2,5-dichloro-1,4-phenylene)bis[4-[[2-chloro-5-(trifluorome	257-776-0	52238-92-3	52238923	3055	Reach_2778	3920	-1.57	3.93	3	4.00									
N,N'-naphthalene-1,5-diylbis[4-[(2,3-dichlorophenyl)azo]-3-hydr	271-178-7	68516-75-6	68516756	3519	Reach_2908	3921	-1.15	3.54	3	4.00									
609-812-5	250-299-9	30693-53-9	30693539	5835	Reach_2649	3922	7.39		1										
3,5-Dihydroxy-4-[3-(4-hydroxyphenyl)propanoyl]phenyl 2-O-(6-d	638-777-9	376348-78-6	376348786	2804	Reach_4601	3923	3.70	0.84	3										
colchicoside	207-513-0	477-29-2	477292	2969	Reach_1290	3924	3.95	2.34	3										
REACH - mono constituent organics (not on SOLUTIONS' MLoS)																			
count							*127*	*103*	*127*	*112*	*102*	*7*	*182*	*182*	*182*	*182*	*182*	*5.5%*	*182*
sum																*6.2%*	*3.2%*	*94.1%*	*0.04%*
standard deviation							*1.34*	*0.41*		*1.393*	*0.44*		*0.9*	*0.9*	*0.9*				
2.5-p													*-6.7*	*-7.0*	*-8.3*	*1.2E-11*	*2.1E-12*		*6.1E-17*
50-p							*4.38*	*0.66*	*3*	*3.30*	*0.67*	*13*	*-4.7*	*-4.9*	*-6.3*	*1.4E-06*	*4.0E-07*		*1.6E-10*
97.5-p													*-3.2*	*-3.5*	*-4.8*	*6.3E-04*	*2.5E-04*		*6.9E-07*
nitrobenzene	202-716-0	98-95-3	98953	-	-	3944	4.55	0.70	56	3.68	0.37		-1.8	-2.0	-3.4	3.66%	2.05%	2.05%	0.03%
2-hydroxy-2-methylpropionitrile	200-909-4	75-86-5	75865	-	-	3945	2.59	0.70	16	1.49	0.70		-2.2	-2.5	-3.8	1.29%	0.66%	2.69%	0.01%
sodium formate	205-488-0	141-53-7	141537	-	-	3946	6.14	0.36	3	5.26	0.47		-2.8	-3.0	-4.4	0.28%	0.13%	2.82%	0.00%
tris[2-[2-(2-methoxyethoxy)ethoxy]ethyl] orthoborate	250-418-4	30989-05-0	30989050	-	-	3947	5.81	0.49	3	4.81	0.49		-2.8	-3.1	-4.5	0.22%	0.10%	2.91%	0.00%
sodium acetate	204-823-8	127-09-3	127093	-	-	3948	6.83	0.23	3	5.83	0.23		-3.2	-3.5	-4.8	0.06%	0.03%	2.93%	0.00%
29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32 copper	205-685-1	147-14-8	147148	-	-	3949	5.40		2	3.00			-3.2	-3.5	-4.8	0.06%	0.02%	2.96%	0.00%
triethylaluminium	202-619-3	97-93-8	97938	-	-	3950	2.69	0.97	3	2.17	0.69		-3.3	-3.5	-4.9	0.06%	0.02%	2.98%	0.00%
benzoyl chloride	202-710-8	98-88-4	98884	-	-	3951	4.56	0.79	5	3.56	0.75		-3.3	-3.5	-4.9	0.05%	0.02%	3.00%	0.00%
1,2-dichlorobenzene	202-425-9	95-50-1	95501	-	-	3952	3.94	0.57	34	2.67	0.12	3	-3.3	-3.5	-4.9	0.05%	0.02%	3.02%	0.00%
Coke (coal), naphtha cracking ethylene manuf. by-product	305-500-5	94581-02-9	94581029	-	-	3953							-3.3	-3.5	-4.9	0.05%	0.02%	3.04%	0.00%
calcium 3-hydroxy-4-[(4-methyl-2-sulphonatophenyl)azo]-2-napl	226-109-5	5281-04-9	5281049	-	-	3954	5.11	0.45	3	3.99	0.64		-3.3	-3.6	-4.9	0.05%	0.02%		0.00%
(+)-tartaric acid	201-766-0	87-69-4	87694	-	-	3955	6.66	1.60	3	5.66	1.60		-3.3	-3.6	-4.9	0.04%	0.02%		0.00%
hydrazine	206-114-9	302-01-2	302012	-	-	3956	2.83	0.66	17	1.83	0.66	17	-3.3	-3.6	-4.9	0.04%	0.02%		0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
N,N-dimethylacetamide	204-826-4	127-19-5	127195	-	-	3957	6.40	0.71	3	5.40	0.70		-3.3	-3.6	-4.9	0.04%	0.02%	0.00%
tributyltin chloride	215-958-7	1461-22-9	1461229	-	-	3958	0.91	0.87	37	-1.21	0.95	10	-3.3	-3.6	-4.9	0.04%	0.02%	0.00%
3,4-dichloroaniline	202-448-4	95-76-1	95761	-	-	3959	3.60	0.60	35	1.92	0.89	13	-3.4	-3.6	-5.0	0.04%	0.02%	0.00%
potassium acetate	204-822-2	127-08-2	127082	-	-	3960	5.85	0.83	3	5.64	0.31		-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
butyllithium	203-698-7	109-72-8	109728	-	-	3961	4.71	0.57	3	3.71	0.57		-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
triethyldialuminium trichloride	235-137-7	12075-68-2	12075682	-	-	3962							-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
2-ethylhexyl 10-ethyl-4,4-dimethyl-7-oxo-8-oxa-3,5-dithia-4-stan	260-829-0	57583-35-4	57583354	-	-	3963	4.83	0.46	3	3.83	0.46		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
2-ethylhexyl 10-ethyl-4-[[2-[(2-ethylhexyl)oxy]-2-oxoethyl]thio]-4	260-828-5	57583-34-3	57583343	-	-	3964	3.48	0.39	3	2.48	0.39		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
1,2-dichloro-4-(trichloromethyl)benzene	235-869-7	13014-24-9	13014249	-	-	3965	4.81		1				-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
pyridine-2-thiol 1-oxide, sodium salt	223-296-5	3811-73-2	3811732	-	-	3966	2.96	1.58	3	2.06	1.64		-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stanna	239-622-4	15571-58-1	15571581	-	-	3967	3.09	1.21	3	2.09	1.21		-3.7	-4.0	-5.3	0.01%	0.00%	0.00%
tetrakis(tritolyl phosphite)nickel	252-777-2	35884-66-3	35884663	-	-	3968	5.50		3	4.50			-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
N-vinylformamide	236-102-9	13162-05-5	13162055	-	-	3969	4.93	0.70	3	3.93	0.70		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
1-isopropyl-2,2-dimethyltrimethylene diisobutyrate	229-934-9	6846-50-0	6846500	-	-	3970	3.87	0.21	3	2.87	0.21		-3.8	-4.1	-5.4	0.01%	0.00%	0.00%
copper chlorophthalocyanine	235-476-0	12239-87-1	12239871	-	-	3971	5.40		2	3.00			-3.8	-4.1	-5.5	0.01%	0.00%	0.00%
sec-butyllithium	209-927-7	598-30-1	598301	-	-	3972	4.94	0.35	3	3.94	0.35		-3.9	-4.1	-5.5	0.01%	0.00%	0.00%
2-ethylhexyl 10-ethyl-4-[[2-[(2-ethylhexyl)oxy]-2-oxoethyl]thio]-4	248-227-6	27107-89-7	27107897	-	-	3973	3.47	1.22	3	2.15	1.52		-3.9	-4.1	-5.5	0.01%	0.00%	0.00%
tetrabutyltin	215-960-8	1461-25-2	1461252	-	-	3974	2.52	0.90	7	1.52	1.06		-3.9	-4.1	-5.5	0.01%	0.00%	0.00%
titanium tetraisopropanolate	208-909-6	546-68-9	546689	-	-	3975	6.13	0.64	3	5.13	0.64		-3.9	-4.1	-5.5	0.01%	0.00%	0.00%
methyl salicylate	204-317-7	119-36-8	119368	-	-	3976	4.90	1.14	3	3.90	1.14		-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
dicyclohexylamine	202-980-7	101-83-7	101837	-	-	3977	4.31	0.78	4	3.00	0.70		-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
tetraethyllead	201-075-4	78-00-2	78002	-	-	3978	2.23	1.14	11	1.23	1.14	11	-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
zinc dilaurate	219-518-5	2452-01-9	2452019	-	-	3979	2.93	0.58	3	1.89	0.67		-3.9	-4.2	-5.6	0.00%	0.00%	0.00%
sodium diethyldithiocarbamate	205-710-6	148-18-5	148185	-	-	3980	3.28	0.31	7	2.28	0.31		-4.0	-4.2	-5.6	0.00%	0.00%	0.00%
n-butyltin trichloride	214-263-6	1118-46-3	1118463	-	-	3981	4.26	1.17	4	3.26	1.06		-4.0	-4.2	-5.6	0.00%	0.00%	0.00%
tetraoctyltin	222-733-7	3590-84-9	3590849	-	-	3982	2.11		1	1.83			-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
sodium hydrogen di(acetate)	204-814-9	126-96-5	126965	-	-	3983	5.63	0.79	3	5.45	0.60		-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
tert-butyl 2-ethylperoxyhexanoate	221-110-7	3006-82-4	3006824	-	-	3984	3.48	0.77	3	2.48	0.77		-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
lithiumbis(trimethylsilyl)amide	223-725-6	4039-32-1	4039321	-	-	3985	5.10	0.49	3	4.10	0.49		-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
bis(triphenylsilyl) chromate	216-612-8	1624-02-8	1624028	-	-	3986							-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
lithium diisopropylamide	223-893-0	4111-54-0	4111540	-	-	3987	5.03	0.42	3	4.03	0.42		-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
dichlorodioctylstannane	222-583-2	3542-36-7	3542367	-	-	3988	3.90		1	2.83			-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
zinc bis(diethyldithiocarbamate)	238-270-9	14324-55-1	14324551	-	-	3989	2.73	0.23	6	1.73	0.23		-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
zinc bis(dibutyldithiocarbamate)	205-232-8	136-23-2	136232	-	-	3990	3.35	1.87	3	2.35	1.87		-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
tin bis(2-ethylhexanoate)	206-108-6	301-10-0	301100	-	-	3991	4.42	0.97	3	3.42	0.97		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
methoxyacetic acid	210-894-6	625-45-6	625456	-	-	3992	4.88	0.70	16	3.88	0.70		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
tributylaluminium	214-240-0	1116-70-7	1116707	-	-	3993							-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
phenyllithium	209-720-1	591-51-5	591515	-	-	3994							-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
bis(2-(2-butoxyethoxy)ethoxy)methane	205-598-9	143-29-3	143293	-	-	3995	5.26	0.42	3	3.91	0.24		-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
2-ethylhexyl 4,4-dibutyl-10-ethyl-7-oxo-8-oxa-3,5-dithia-4-stann	234-186-1	10584-98-2	10584982	-	-	3996	2.90	1.24	3	1.90	1.24		-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
dibutyltin oxide	212-449-1	818-08-6	818086	-	-	3997	3.16	0.19	3	2.16	0.19		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
ammonium acetate	211-162-9	631-61-8	631618	-	-	3998	5.99	0.62	3	4.99	0.62		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
dibutyltin dichloride	211-670-0	683-18-1	683181	-	-	3999	2.47	1.00	7	2.90	2.65		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
N-[3-(dimethylamino)propyl]methacrylamide	226-002-3	5205-93-6	5205936	-	-	4000	5.27	0.31	3	4.47	0.28		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
imidazole	206-019-2	288-32-4	288324	-	-	4001	5.37	0.22	3	4.37	0.22		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
trichlorooctylstannane	221-435-4	3091-25-6	3091256	-	-	4002	2.33		1				-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
sodium dibenzyldithiocarbamate	259-587-9	55310-46-8	55310468	-	-	4003	3.05		2				-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
aluminium triformate	230-898-1	7360-53-4	7360534	-	-	4004	3.11	0.70	3	2.11	0.70		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
sodium (S)-lactate	212-762-3	867-56-1	867561	-	-	4005	6.07	0.83	3	5.51	0.72		-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
2-(2H-benzotriazol-2-yl)-p-cresol	219-470-5	2440-22-4	2440224	-	-	4006	4.34	1.40	3	3.34	1.40		-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
diethylaluminium chloride	202-477-2	96-10-6	96106	-	-	4007							-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
dioctyltin oxide	212-791-1	870-08-6	870086	-	-	4008							-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
diethylzinc	209-161-3	557-20-0	557200	-	-	4009							-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
2,4-dichloro-1-(trichloromethyl)benzene	235-868-1	13014-18-1	13014181	-	-	4010	5.12	0.23	3	4.12	0.23		-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
diisobutylaluminium hydride	214-729-9	1191-15-7	1191157	-	-	4011							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
lead di(acetate)	206-104-4	301-04-2	301042	-	-	4012	3.90	0.70	18	2.90	0.70	18	-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
benzylmagnesium chloride	230-039-0	6921-34-2	6921342	-	-	4013							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
614-695-9	614-695-9	68649-12-7	68649127	-	-	4014	6.46	0.14	3	5.46	0.14		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
4-(Pyridin-4-yl)-1,3-thiazole-2(3H)-thione	616-441-2	77168-63-9	77168639	-	-	4015							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
(2-hydroxyethyl)(3-hydroxypropyl)dimethylammonium chloride	278-860-3	78182-00-0	78182000	-	-	4016							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
trichloro(chloromethyl)silane	216-316-9	1558-25-4	1558254	-	-	4017							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
2-fluorotoluene	202-428-5	95-52-3	95523	-	-	4018	4.29		1				-4.4	-4.7	-6.0	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
di(morpholin-4-yl) disulphide	203-103-0	103-34-4	103344	-	-	4019	3.94	0.50	3	2.94	0.50		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
magnesium ethanolate	219-323-5	2414-98-4	2414984	-	-	4020	6.41	0.72	3	5.85	1.25		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
3-aminopropyldiethylamine	203-236-4	104-78-9	104789	-	-	4021	5.10	0.98	3	4.24	1.06		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
tricarbonyl(methylcyclopentadienyl)manganese	235-166-5	12108-13-3	12108133	-	-	4022	2.73	0.35	3	1.73	0.35		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
zinc bis[12-hydroxyoctadecanoate]	252-669-5	35674-68-1	35674681	-	-	4023	2.93	0.58	3	1.89	0.67		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
ferrocene	203-039-3	102-54-5	102545	-	-	4024	3.60	0.54	3	2.48	0.99		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
ethyl 9,9-dioctyl-4,7,11-trioxo-3,8,10-trioxa-9-stannatetradeca-5	268-500-3	68109-88-6	68109886	-	-	4025							-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
Lead titanium zirconium oxide	235-727-4	12626-81-2	12626812	-	-	4026	2.32	0.52	3	1.32	0.52		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
dibutyltin dilaurate	201-039-8	77-58-7	77587	-	-	4027	2.98		2				-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
titanium(4+) ethanolate	221-410-8	3087-36-3	3087363	-	-	4028	6.73	0.57	4	5.59	0.66		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
ethylaluminium dichloride	209-248-6	563-43-9	563439	-	-	4029							-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
[2R-(2α,3Z,5α)]-3-(2-hydroxyethylidene)-7-oxo-4-oxa-1-azabicycl	266-104-5	66069-34-9	66069349	-	-	4030	5.77	0.95	3	4.77	0.95		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
adipohydrazide	213-999-5	1071-93-8	1071938	-	-	4031	5.03	0.82	3	4.03	0.82		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
bis(2,4-dichlorobenzoyl) peroxide	205-094-9	133-14-2	133142	-	-	4032							-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
sodium lactate	200-772-0	72-17-3	72173	-	-	4033	5.75	0.50	3	5.14	0.48		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
bismuth oxide salicylate	238-953-1	14882-18-9	14882189	-	-	4034							-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
copper di(acetate)	205-553-3	142-71-2	142712	-	-	4035	2.68	0.60	5	1.35	0.39		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
aluminium triisopropanolate	209-090-8	555-31-7	555317	-	-	4036	4.17	2.00	3	3.49	1.74		-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
sodium dihydridobis(2-methoxyethanolato)aluminate(1-)	245-178-2	22722-98-1	22722981	-	-	4037							-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
(R*,R*)-(±)-5-amino-N,N'-bis(2,3-dihydroxypropyl)-2,4,6-triiodois	266-162-1	66108-89-2	66108892	-	-	4038	5.50		3	4.50			-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
titanium(4+) 2-(dimethylamino)ethanolate	257-897-9	52406-71-0	52406710	-	-	4039	4.80		1				-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
2,2-dioctyl-1,3,2-oxathiastannolan-5-one	239-581-2	15535-79-2	15535792	-	-	4040							-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
2-(2H-benzotriazol-2-yl)-4,6-ditertpentylphenol	247-384-8	25973-55-1	25973551	-	-	4041							-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
lactic acid, compound with 3-[2-(dimethylamino)ethyl] 1-(2-ethy	269-358-5	68227-46-3	68227463	-	-	4042	2.91		2	2.56			-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
magnesium di(acetate)	205-554-9	142-72-3	142723	-	-	4043	6.20	0.27	3	5.20	0.27		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
sodium piperidine-1-carbodithioate	212-843-3	873-57-4	873574	-	-	4044							-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
titanium tetrakis(2-ethylhexanolate)	213-969-1	1070-10-6	1070106	-	-	4045	4.38	0.30	3	3.38	0.30		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
[1,3,8,16,18,24-hexabromo-2,4,9,10,11,15,17,22,23,25-decachlo	238-238-4	14302-13-7	14302137	-	-	4046	5.40		2	3.00			-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
N-(3-aminopropyl)iminodiethanol	225-642-0	4985-85-7	4985857	-	-	4047	3.79		1				-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
617-903-6	617-903-6	86675-46-9	86675469	-	-	4048							-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
cyclohex-3-ene-1-carbaldehyde	202-858-3	100-50-5	100505	-	-	4049	4.69		2				-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
aluminium tri-sec-butanolate	218-871-2	2269-22-9	2269229	-	-	4050	4.43	1.77	3	3.22	1.62		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
triisobutylaluminium	202-906-3	100-99-2	100992	-	-	4051							-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
methyl (Z,Z)-8,8-dibutyl-3,6,10-trioxo-2,7,9-trioxa-8-stannatridec	239-594-3	15546-11-9	15546119	-	-	4052	3.39	0.56	3	2.53	0.58		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
p-methoxypropiophenone	204-512-7	121-97-1	121971	-	-	4053							-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
trisodium bis[2-[[2,4-dihydroxy-3-[(2-methyl-4-sulphophenyl)azo	278-145-6	75234-41-2	75234412	-	-	4054	4.99	0.62	3	3.99	0.62		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
phenylacetic acid	203-148-6	103-82-2	103822	-	-	4055	4.84	0.78	4	3.84	0.78		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
619-419-0	619-419-0	99290-97-8	99290978	-	-	4056							-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
1,3-diethyldiphenylurea	201-645-2	85-98-3	85983	-	-	4057	4.14	0.42	3	3.23	0.48		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
trioctylaluminium	213-964-4	1070-00-4	1070004	-	-	4058							-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
calcium (S)-2-hydroxypropionate	248-953-3	28305-25-1	28305251	-	-	4059	5.98	0.78	3	5.78	0.66		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
Phosphorous acid, tri-C12-14-alkyl esters	297-701-9	93686-48-7	93686487	-	-	4060	5.53	1.42	3	4.53	1.42		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
bis(ethyl acetoacetato-O1',O3)bis(2-methylpropan-1-olato)titani	281-161-6	83877-91-2	83877912	-	-	4061	6.09	0.36	3	5.09	0.36		-5.0	-5.3	-6.7	0.00%	0.00%	0.00%
[29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]zinc	238-262-5	14320-04-8	14320048	-	-	4062							-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
bis(ethyl acetoacetato-O1',O3)bis(propan-2-olato)titanium	248-697-2	27858-32-8	27858328	-	-	4063	5.84	0.98	3	4.84	0.98		-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
3-[(4-chloro-2-nitrophenyl)azo]-2-methylpyrazolo[5,1-b]quinazol	277-823-9	74336-59-7	74336597	-	-	4064							-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
trichlorotrimethyldialuminium	235-698-8	12542-85-7	12542857	-	-	4065							-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
dimethyltin dichloride	212-039-2	753-73-1	753731	-	-	4066	3.23	1.75	7	2.23	1.06		-5.1	-5.4	-6.8	0.00%	0.00%	0.00%
ferrate(4-), hexakis(cyano-C)-, methylated 4-[(4-aminophenyl)(4-	235-468-7	12237-62-6	12237626	-	-	4067	3.88		2				-5.1	-5.4	-6.8	0.00%	0.00%	0.00%
N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2-met	235-425-2	12225-06-8	12225068	-	-	4068	4.17	1.05	3	3.17	1.05		-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
bismuth citrate	212-390-1	813-93-4	813934	-	-	4069							-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
dibutylbis(pentane-2,4-dionato-O,O')tin	245-152-0	22673-19-4	22673194	-	-	4070	2.95	1.47	3	1.95	1.47		-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
butylethylmagnesium	263-454-0	62202-86-2	62202862	-	-	4071							-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
Octanoic acid, zinc salt, basic	291-793-4	90480-58-3	90480583	-	-	4072	2.45	0.41	3	1.89	0.67		-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
tin(II) oxalate	212-414-0	814-94-8	814948	-	-	4073	5.17	0.05	3	4.17			-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
Amides, tall-oil fatty, N-(hydroxyethyl)	268-950-0	68155-22-6	68155226	-	-	4074							-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]	276-461-9	72207-62-6	72207626	-	-	4075	5.26	1.21	3	4.26	1.21		-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
[phthalato(2-)]dioxotrilead	273-688-5	69011-06-9	69011069	-	-	4076	2.43	0.68	3	2.06	0.70		-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
dichloroisobutylaluminium	217-563-5	1888-87-5	1888875	-	-	4077							-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
601-495-1	601-495-1	117829-74-0	117829740	-	-	4078							-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
dipropylmalonic acid	216-664-1	1636-27-7	1636277	-	-	4079							-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
696-062-7	696-062-7	14878-28-5	14878285	-	-	4080							-5.2	-5.5	-6.9	0.00%	0.00%	0.00%

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aluminium tri(hexanolate)	245-546-2	23275-26-5	23275265	-	-	4081							-5.2	-5.5	-6.9	0.00%	0.00%		0.00%
619-741-1	619-741-1	874209-13-9	874209139	-	-	4082							-5.2	-5.5	-6.9	0.00%	0.00%		0.00%
chromium trioleate	244-256-3	21178-63-2	21178632	-	-	4083	5.17		1				-5.2	-5.5	-6.9	0.00%	0.00%		0.00%
3-(4-amino-2-methylpyrimidin-5-ylmethyl)-5-(2-hydroxyethyl)-4-	206-077-9	299-35-4	299354	-	-	4084							-5.2	-5.5	-6.9	0.00%	0.00%		0.00%
605-753-4	605-753-4	175217-23-9	175217239	-	-	4085							-5.2	-5.5	-6.9	0.00%	0.00%		0.00%
Alkanes, C4-12	269-792-5	68333-81-3	68333813	-	-	4086							-5.2	-5.5	-6.9	0.00%	0.00%		0.00%
lead 2,4,6-trinitro-m-phenylene dioxide	239-290-0	15245-44-0	15245440	-	-	4087	2.48	0.67	3	2.03	0.69		-5.3	-5.5	-6.9	0.00%	0.00%		0.00%
trihexylaluminium	214-241-6	1116-73-0	1116730	-	-	4088							-5.3	-5.6	-6.9	0.00%	0.00%		0.00%
sodium 2-methylbutan-2-olate	238-639-4	14593-46-5	14593465	-	-	4089							-5.4	-5.6	-7.0	0.00%	0.00%		0.00%
trimethylaluminium	200-853-0	75-24-1	75241	-	-	4090							-5.4	-5.6	-7.0	0.00%	0.00%		0.00%
magnesium 2-methylpropan-2-olate	250-931-3	32149-57-8	32149578	-	-	4091							-5.4	-5.7	-7.1	0.00%	0.00%		0.00%
citric acid, nickel salt	245-119-0	22605-92-1	22605921	-	-	4092	3.33	1.02	3	2.33	1.02		-5.6	-5.8	-7.2	0.00%	0.00%		0.00%
606-280-6	606-280-6	192704-54-4	192704544	-	-	4093							-5.7	-5.9	-7.3	0.00%	0.00%		0.00%
dibutoxydibutylstannane	222-103-1	3349-36-8	3349368	-	-	4094	3.16	0.17	3	2.16	0.17		-5.7	-5.9	-7.3	0.00%	0.00%		0.00%
dibutyldimethoxystannane	213-935-6	1067-55-6	1067556	-	-	4095	3.55	0.27	3	2.55	0.27		-5.7	-5.9	-7.3	0.00%	0.00%		0.00%
4-amino-6-[(E)-{5-[(4-chloro-6-{ethyl[3-(vinylsulfonyl)phenyl]ami	700-419-5	1177247-66-3	1177247663	-	-	4096	5.06	0.26	3	4.06	0.26		-5.7	-6.0	-7.3	0.00%	0.00%		0.00%
dibutyltin maleate	201-077-5	78-04-6	78046	-	-	4097	3.39	0.56	3	2.53	0.58		-5.7	-6.0	-7.3	0.00%	0.00%		0.00%
3-hydroxy-4'-methoxy-2-naphthanilide	202-190-2	92-79-5	92795	-	-	4098							-5.8	-6.0	-7.4	0.00%	0.00%		0.00%
chromium triacetate	213-909-4	1066-30-4	1066304	-	-	4099	5.62		1				-5.8	-6.0	-7.4	0.00%	0.00%		0.00%
bis(tributyltin) oxide	200-268-0	56-35-9	56359	-	-	4100	1.14	1.29	65	-0.13	1.06	18	-5.8	-6.1	-7.4	0.00%	0.00%		0.00%
methylmagnesium chloride	211-629-7	676-58-4	676584	-	-	4101							-5.9	-6.1	-7.5	0.00%	0.00%		0.00%
[2-{[(2-{3-[(4-{ethyl[3-(vinylsulfonyl)phenyl]amino}-6-fluoro-1,3,5	700-687-3	1291070-04-6	1291070046	-	-	4102	5.08	0.68	3	4.08	0.68		-5.9	-6.1	-7.5	0.00%	0.00%		0.00%
diethyl ethyl(1-methylbutyl)malonate	200-981-7	76-72-2	76722	-	-	4103							-5.9	-6.2	-7.5	0.00%	0.00%		0.00%
disodium hydrogen bis[3-hydroxy-4-[(2-hydroxy-1-naphthyl)azo]	235-628-6	12392-64-2	12392642	-	-	4104	4.69	0.30	3	3.69	0.30		-5.9	-6.2	-7.5	0.00%	0.00%		0.00%
trisodium [3-{(E)-[4-{[6-anilino-1-(hydroxy-κO)-3-sulfo-2-naphthy	616-328-8	76359-37-0	76359370	-	-	4105	5.01		2				-6.1	-6.3	-7.7	0.00%	0.00%		0.00%
bis[1-carbamimidoyl-kN'-urea-kO)]copper(2+) dinitrate	800-038-5	1071838-81-7	1071838817	-	-	4106	2.16		2				-6.1	-6.3	-7.7	0.00%	0.00%		0.00%
Magnesium bis(2-ethylbutanoate)	700-021-1	79992-76-0	79992760	-	-	4107	5.41	0.19	3	4.41	0.19		-6.1	-6.4	-7.7	0.00%	0.00%		0.00%
4-[(4-chloro-2-nitrophenyl)azo]-3-hydroxy-N-(2-methylphenyl)na	229-314-8	6471-50-7	6471507	-	-	4108	5.04	1.10	3	4.04	1.10		-6.1	-6.4	-7.7	0.00%	0.00%		0.00%
nickel(2+) hydrogen citrate	242-533-3	18721-51-2	18721512	-	-	4109	3.33	1.02	3	2.33	1.02		-6.1	-6.4	-7.7	0.00%	0.00%		0.00%
cobalt(2+) hydrogen citrate	242-538-0	18727-04-3	18727043	-	-	4110	3.16	0.64	4	3.34	1.13		-6.1	-6.4	-7.7	0.00%	0.00%		0.00%
aluminium tris(2,4-pentanedionato-O,O')	237-741-6	13963-57-0	13963570	-	-	4111	8.14	0.35	3	7.14	0.35		-6.1	-6.4	-7.7	0.00%	0.00%		0.00%
hydrogen [1-[(2-hydroxy-4-nitrophenyl)azo]-2-naphtholato(2-)][	257-804-1	52277-71-1	52277711	-	-	4112							-6.2	-6.4	-7.8	0.00%	0.00%		0.00%
Solvate of methyl 1-C-[4-chloro-3-(4-ethoxybenzyl)phenyl]-D-g	619-496-0	960404-59-5	960404595	-	-	4113	4.77		1				-6.2	-6.4	-7.8	0.00%	0.00%		0.00%
Magnesium bis(2-ethylhexan-1-olate)	805-232-3	98906-78-6	98906786	-	-	4114							-6.2	-6.5	-7.9	0.00%	0.00%		0.00%
1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthyl)ethan-	244-240-6	21145-77-7	21145777	-	-	4115	2.79		1	2.45			-6.3	-6.6	-7.9	0.00%	0.00%		0.00%
chloro(1-methylethyl)magnesium	213-947-1	1068-55-9	1068559	-	-	4116							-6.4	-6.7	-8.0	0.00%	0.00%		0.00%
pyridinium dichromate	243-478-8	20039-37-6	20039376	-	-	4117	2.83		2				-6.6	-6.8	-8.2	0.00%	0.00%		0.00%
trinickel dicitrate	227-873-2	6018-92-4	6018924	-	-	4118	3.33	1.02	3	2.33	1.02		-6.6	-6.8	-8.2	0.00%	0.00%		0.00%
(6R,6'S)-6,6'-ethane-1,2-diylbis(6H-dibenzo[c,e][1,2]oxaphosphir	700-929-8	1337918-51-0	1337918510	-	-	4119	2.84	0.68	3	1.84	0.68		-6.6	-6.8	-8.2	0.00%	0.00%		0.00%
sodium bis[N-[7-hydroxy-8-[[2-hydroxy-5-[(methylamino)sulphoı	273-454-2	68966-87-0	68966870	-	-	4120							-6.6	-6.9	-8.2	0.00%	0.00%		0.00%
Acetic acid, chromium salt, basic	254-447-3	39430-51-8	39430518	-	-	4121							-6.8	-7.1	-8.4	0.00%	0.00%		0.00%
sodium hydrogen (3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phı	700-812-1	1189052-95-6	1189052956	-	-	4122							-6.9	-7.1	-8.5	0.00%	0.00%		0.00%
2-ethylhexyl lactate	228-503-2	6283-86-9	6283869	-	-	4123	4.76	0.59	3	3.76	0.59		-6.9	-7.1	-8.5	0.00%	0.00%		0.00%
612-411-8	612-411-8	61813-75-0	61813750	-	-	4124	4.69	0.55	3	3.69	0.55		-6.9	-7.2	-8.5	0.00%	0.00%		0.00%
tricobalt dicitrate	212-751-3	866-81-9	866819	-	-	4125	2.97	0.42	4	1.97	0.42		-7.2	-7.4	-8.8	0.00%	0.00%		0.00%
REACH - UVCB organics (not on SOLUTIONS' MLoS)																			
count							*914*	*748*	*914*	*824*	*745*	*4*	*1144*	*1144*	*1144*	*1144*	*1144*	*8.6%*	*1144*
sum																*66%*	*44%*	*91.4%*	*1.1%*
standard deviation							*1.19*	*0.50*		*1.191*	*0.53*		*0.9*	*0.9*	*0.9*				
2.5-p													*-6.2*	*-6.5*	*-7.8*	*2.7E-10*	*5.3E-11*		*2.9E-15*
50-p							*4.52*	*0.59*	*3*	*3.64*	*0.63*	*12*	*-4.5*	*-4.7*	*-6.1*	*4.0E-06*	*1.2E-06*		*6.6E-10*
97.5-p													*-2.4*	*-2.7*	*-4.0*	*7.3E-03*	*3.6E-03*		*2.6E-05*
Fatty acids, C16-18 and C18-unsatd., Me esters	267-015-4	67762-38-3	67762383	-	-	4127	6.47	2.97	3	5.47	2.97		-1.2	-1.5	-2.8	10.93%	6.92%	6.9%	0.23%
Fatty acids, vegetable-oil, Me esters	273-606-8	68990-52-3	68990523	-	-	4128	6.47	2.97	3	5.47	2.97		-1.3	-1.5	-2.9	10.13%	6.36%	12.8%	0.20%
618-882-6	618-882-6	928771-01-1	928771011	-	-	4129							-1.4	-1.6	-3.0	8.18%	5.00%	17.2%	0.14%
Hydrocarbons, C4	289-339-5	87741-01-3	87741013	-	-	4130	4.33	0.32	3	3.33	0.32		-1.5	-1.7	-3.1	7.03%	4.23%	20.7%	0.10%
Fatty acids, C14-18 and C16-18-unsatd., Me esters	267-007-0	67762-26-9	67762269	-	-	4131	6.47	2.97	3	5.47	2.97		-1.7	-1.9	-3.3	4.78%	2.75%	22.9%	0.05%
Light oil (coal), coke-oven	266-012-5	65996-78-3	65996783	-	-	4132	3.90	0.39	5	2.90	0.39		-1.7	-2.0	-3.3	4.42%	2.53%	24.8%	0.05%
Fatty acids, C10-18 and C12-22-unsatd., C14-18 and C16-18-unsa	285-200-8	85049-31-6	85049316	-	-	4133	6.47	2.97	3	5.47	2.97		-1.8	-2.1	-3.4	3.57%	1.99%	26.3%	0.03%
Tar, coal, high-temp.	266-024-0	65996-89-6	65996896	-	-	4134	4.32	0.27	3	3.62	0.59		-1.8	-2.1	-3.4	3.52%	1.97%	27.8%	0.03%
Hydrocarbons, C3-4	270-681-9	68476-40-4	68476404	-	-	4135	4.41	0.39	3	3.41	0.39		-1.9	-2.2	-3.5	2.80%	1.53%	28.9%	0.02%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]		TP(Cwcoast) [-]
Pitch, coal tar, high-temp.	266-028-2	65996-93-2	65996932	-	-	4136	4.34	2.21	3	4.88	1.26		-1.9	-2.2	-3.5	2.63%	1.43%	29.9%	0.02%
Formaldehyde, oligomeric reaction products with aniline and ph	500-079-6	32055-14-4	32055144	-	-	4137	6.37	0.26	3	5.37	0.26		-1.9	-2.2	-3.5	2.60%	1.41%	30.9%	0.02%
Petroleum gases, liquefied, sweetened	270-705-8	68476-86-8	68476868	-	-	4138	4.41	0.39	3	3.41	0.39		-2.0	-2.2	-3.6	2.56%	1.38%	31.8%	0.02%
Formaldehyde, oligomeric reaction products with aniline	500-036-1	25214-70-4	25214704	-	-	4139	3.78	0.70	3	2.78	0.70		-2.1	-2.3	-3.7	1.90%	1.00%	32.5%	0.01%
Charcoal	240-383-3	16291-96-6	16291966	4995	PharmaBeta_418	4140	4.53	0.41	3				-4.6	-4.0	-6.2	0.00%	0.00%	32.5%	0.00%
Benzene, C10-13-alkyl derivs.	267-051-0	67774-74-7	67774747	-	-	4141	2.00		1	1.03			-2.1	-2.4	-3.7	1.61%	0.84%	33.1%	0.01%
Naphtha (petroleum), light steam-cracked, thermally treated	308-714-7	98219-47-7	98219477	-	-	4142	3.30	0.22	3	2.30	0.22		-2.2	-2.4	-3.8	1.56%	0.80%	33.6%	0.01%
m-tolylidene diisocyanate	247-722-4	26471-62-5	26471625	-	-	4143	5.50	1.31	3	4.50	1.31		-2.2	-2.4	-3.8	1.47%	0.76%	34.1%	0.01%
dinitrotoluene	246-836-1	25321-14-6	25321146	-	-	4144	3.99	0.59	3	2.79	0.72		-2.2	-2.5	-3.8	1.27%	0.65%	34.6%	0.01%
Benzenesulfonic acid, 4-C10-13-sec-alkyl derivs.	287-494-3	85536-14-7	85536147	-	-	4145	3.67	0.53	4	3.13	0.51		-2.3	-2.5	-3.9	1.20%	0.61%	35.0%	0.01%
Distillates (coal tar), heavy oils	292-607-4	90640-86-1	90640861	-	-	4146	4.77	0.35	3	3.71	0.97		-2.3	-2.5	-3.9	1.18%	0.60%	35.3%	0.01%
Tall oil, sodium salt	266-037-1	65997-01-5	65997015	-	-	4147	5.01	0.61	3	3.70	0.70		-2.3	-2.5	-3.9	1.11%	0.56%	35.7%	0.01%
Alcohols, C12-14, ethoxylated, sulfates, sodium salts	500-234-8	68891-38-3	68891383	-	-	4148	3.72	0.46	3	2.72	0.46		-2.3	-2.5	-3.9	1.09%	0.54%	36.1%	0.00%
diaminotoluene	246-910-3	25376-45-8	25376458	-	-	4149	4.12	1.23	3	3.12	1.23		-2.3	-2.5	-3.9	1.08%	0.54%	36.4%	0.00%
Naphtha (petroleum), light steam-cracked, debenzenized	271-266-5	68527-26-4	68527264	-	-	4150	3.30	0.22	3	2.30	0.22		-2.3	-2.6	-3.9	1.06%	0.53%	36.7%	0.00%
Alcohols, C12-14, ethoxylated	500-213-3	68439-50-9	68439509	-	-	4151	3.12	0.47	4	2.24	0.50		-2.3	-2.6	-3.9	0.96%	0.47%	37.0%	0.00%
Rosin	232-475-7	8050-09-7	8050097	-	-	4152	4.09	1.16	3	3.77	1.29		-2.4	-2.6	-4.0	0.93%	0.46%	37.3%	0.00%
Distillates (coal tar), naphthalene oils	283-484-8	84650-04-4	84650044	-	-	4153	4.87	0.89	3	3.87	0.89		-2.4	-2.6	-4.0	0.90%	0.45%	37.6%	0.00%
Tall-oil pitch	232-414-4	8016-81-7	8016817	-	-	4154	6.05	0.41	3	5.05	0.41		-2.4	-2.7	-4.0	0.79%	0.39%	37.8%	0.00%
Ascophyllum nodosum, ext.	283-907-6	84775-78-0	84775780	-	-	4155	5.34	0.31	3	4.34	0.31		-2.4	-2.7	-4.0	0.76%	0.37%	38.1%	0.00%
Shale oils	269-646-0	68308-34-9	68308349	-	-	4156	3.97	0.38	3	2.97	0.38		-2.4	-2.7	-4.0	0.76%	0.37%	38.3%	0.00%
Fatty acids, C16-18	266-928-5	67701-03-5	67701035	-	-	4157							-2.4	-2.7	-4.1	0.72%	0.35%	38.5%	0.00%
308065-15-8	629-776-4	308065-15-8	308065158	-	-	4158	6.23		1	5.00			-2.5	-2.7	-4.1	0.66%	0.31%	38.7%	0.00%
Benzenesulfonic acid, C10-13-alkyl derivs., sodium salts	270-115-0	68411-30-3	68411303	-	-	4159	3.62	0.51	6	3.13	0.51		-2.5	-2.7	-4.1	0.64%	0.30%	38.9%	0.00%
Alkenes, C10-13	287-479-1	85535-87-1	85535871	-	-	4160	2.96	0.82	3	3.44	2.00		-2.5	-2.8	-4.1	0.58%	0.28%	39.1%	0.00%
Hydrocarbons, C5-8	295-762-6	92128-65-9	92128659	-	-	4161	3.70	0.48	3	2.70	0.48		-2.5	-2.8	-4.1	0.57%	0.27%	39.2%	0.00%
Anthracene oil	292-602-7	90640-80-5	90640805	-	-	4162	4.77	0.35	3	3.71	0.97		-2.5	-2.8	-4.1	0.56%	0.26%	39.4%	0.00%
Fatty acids, C8-18 and C18-unsatd., Me esters	267-014-9	67762-37-2	67762372	-	-	4163	2.41		2	2.12			-2.5	-2.8	-4.1	0.55%	0.26%	39.5%	0.00%
Lubricating oils, used	274-635-9	70514-12-4	70514124	-	-	4164	6.29	1.09	3	5.29	1.09		-2.5	-2.8	-4.1	0.55%	0.26%	39.7%	0.00%
Wheat, ext., hydrolyzed	309-358-5	100209-50-5	100209505	-	-	4165	5.00		1				-2.6	-2.8	-4.2	0.48%	0.23%	39.8%	0.00%
1,2-Benzenedicarboxylic acid, di-C9-11-branched alkyl esters, C1	271-091-4	68515-49-1	68515491	-	-	4166	3.34	0.74	3	2.34	0.74		-2.6	-2.9	-4.2	0.43%	0.20%	40.0%	0.00%
Tall oil	232-304-6	8002-26-4	8002264	-	-	4167	5.15	1.54	3	4.80	1.31		-2.6	-2.9	-4.2	0.42%	0.20%	40.1%	0.00%
Alcohols, C9-11-iso-, C10-rich	271-234-0	68526-85-2	68526852	-	-	4168	3.53	0.13	3	2.53	0.13		-2.7	-2.9	-4.3	0.38%	0.18%		0.00%
Charcoal, coconut shell	271-974-4	68647-86-9	68647869	-	-	4169							-2.7	-3.0	-4.3	0.31%	0.14%		0.00%
1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9	271-090-9	68515-48-0	68515480	-	-	4170	3.72	0.88	3	2.72	0.88		-2.7	-3.0	-4.3	0.30%	0.14%		0.00%
Fatty acids, C14-18 and C16-18-unsatd.	266-930-6	67701-06-8	67701068	-	-	4171	5.67	0.38	3	4.92	0.75		-2.8	-3.0	-4.4	0.29%	0.13%		0.00%
Creosote oil, acenaphthene fraction	292-605-3	90640-84-9	90640849	-	-	4172	3.94	0.95	3	3.10	1.00		-2.8	-3.0	-4.4	0.29%	0.13%		0.00%
Alcohols, C8-10-iso-, C9-rich	271-233-5	68526-84-1	68526841	-	-	4173	3.96	0.16	3	3.26	0.20		-2.8	-3.0	-4.4	0.28%	0.13%		0.00%
Corn, steep liquor	266-113-4	66071-94-1	66071941	-	-	4174	4.77	0.56	3	3.98	0.95		-2.8	-3.0	-4.4	0.28%	0.12%		0.00%
Syrups, corn, hydrogenated	270-337-8	68425-17-2	68425172	-	-	4175							-2.8	-3.0	-4.4	0.28%	0.12%		0.00%
Dec-1-ene, homopolymer, hydrogenated Dec-1-ene, oligomers,	500-183-1	68037-01-4	68037014	-	-	4176	6.46	0.14	3	5.46	0.14		-2.8	-3.0	-4.4	0.27%	0.12%		0.00%
Benzene, (1-methylethyl)-, oxidized, polyphenyl residues	269-798-8	68333-89-1	68333891	-	-	4177	4.93		2				-2.8	-3.0	-4.4	0.27%	0.12%		0.00%
Alkanes, C14-17, chloro	287-477-0	85535-85-9	85535859	-	-	4178	3.16	1.40	3	2.16	1.40		-2.8	-3.0	-4.4	0.26%	0.12%		0.00%
Distillates (petroleum), steam-cracked	265-194-3	64742-91-2	64742912	-	-	4179	3.30	0.22	3	2.30	0.22		-2.8	-3.1	-4.4	0.25%	0.11%		0.00%
Tar, brown-coal, low-temp.	309-886-6	101316-84-1	101316841	-	-	4180	4.41	0.15	3	3.61	0.25		-2.8	-3.1	-4.4	0.25%	0.11%		0.00%
Sucrose, propoxylated	500-029-3	9049-71-2	9049712	-	-	4181	6.48	0.97	3	5.48	0.97		-2.8	-3.1	-4.4	0.24%	0.11%		0.00%
vinyl neodecanoate	256-905-8	51000-52-3	51000523	-	-	4182	3.32	0.91	3	2.32	0.91		-2.8	-3.1	-4.4	0.24%	0.11%		0.00%
629-693-3	629-693-3	740817-83-8	740817838	-	-	4183	3.00	0.63	3	2.00	0.63		-2.8	-3.1	-4.4	0.23%	0.10%		0.00%
Fatty acids, C6-24 and C6-24-unsatd., Me esters, distn. residues	310-083-8	102242-52-4	102242524	-	-	4184	5.83	1.53	3	4.83	1.53		-2.9	-3.1	-4.5	0.22%	0.10%		0.00%
D-Glucitol, propoxylated	500-118-7	52625-13-5	52625135	-	-	4185				4.00			-2.9	-3.1	-4.5	0.22%	0.10%		0.00%
Hydrocarbons, C5, ethylene-manuf.-by-product, hydrogenated	295-765-2	92128-68-2	92128682	-	-	4186	4.07	0.39	3	3.07	0.39		-2.9	-3.1	-4.5	0.21%	0.09%		0.00%
Glycerol, propoxylated	500-044-5	25791-96-2	25791962	-	-	4187				4.00			-2.9	-3.1	-4.5	0.21%	0.09%		0.00%
615-494-9	615-494-9	71808-39-4	71808394	-	-	4188	6.07	1.05	3	5.07	1.05		-2.9	-3.1	-4.5	0.20%	0.09%		0.00%
Amines, C12-14-alkyldimethyl	283-464-9	84649-84-3	84649843	-	-	4189	2.12	0.66	3	1.18	0.77		-2.9	-3.1	-4.5	0.20%	0.09%		0.00%
Soybean oil, epoxidized	232-391-0	8013-07-8	8013078	-	-	4190	5.04	1.51	3	4.04	1.51		-2.9	-3.1	-4.5	0.19%	0.08%		0.00%
Fatty acids, C18-unsatd., dimers	500-148-0	61788-89-4	61788894	-	-	4191				2.93			-2.9	-3.2	-4.5	0.17%	0.07%		0.00%
Ethers, C5-6-branched alkyl Me	295-322-3	91995-60-7	91995607	-	-	4192	5.33	0.64	3	4.33	0.64		-2.9	-3.2	-4.6	0.16%	0.07%		0.00%
Pitch, petroleum, arom.	269-110-6	68187-58-6	68187586	-	-	4193	4.73	2.93	3	3.73	2.93		-3.0	-3.2	-4.6	0.15%	0.06%		0.00%
Distillates (petroleum), C3-6, piperylene-rich	270-726-2	68477-35-0	68477350	-	-	4194	4.07	0.39	3	3.07	0.39		-3.0	-3.2	-4.6	0.15%	0.06%		0.00%
(1-methyl-1,2-ethanediyl)bis[oxy(methyl-2,1-ethanediyl)] diacryl	256-032-2	42978-66-5	42978665	-	-	4195	4.53	0.61	3	3.48	0.75		-3.0	-3.2	-4.6	0.15%	0.06%		0.00%
Butene, homopolymer (products derived from either/or But-1-e	500-004-7	9003-29-6	9003296	-	-	4196	1.72	0.19	3	0.72	0.19		-3.0	-3.2	-4.6	0.14%	0.06%		0.00%
Cyclohexane, oxidized, aq. ext.	272-810-4	68915-38-8	68915388	-	-	4197	5.47	0.33	3	4.47	0.33		-3.0	-3.2	-4.6	0.14%	0.06%		0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Fatty acids, C8-18 and C18-unsatd.	266-929-0	67701-05-7	67701057	-	-	4198	4.49	1.59	3	3.49	1.59		-3.0	-3.3	-4.6	0.13%	0.06%	0.00%
Turpentine, oil	232-350-7	8006-64-2	8006642	-	-	4199	4.20	0.27	3	3.13	0.31		-3.0	-3.3	-4.6	0.13%	0.06%	0.00%
Sulfuric acid, mono-C12-14-alkyl esters, sodium salts	287-809-4	85586-07-8	85586078	-	-	4200	3.91	0.57	3	2.89	0.36		-3.0	-3.3	-4.6	0.13%	0.06%	0.00%
Benzene, mono-C10-13-alkyl derivs., distn. residues	284-660-7	84961-70-6	84961706	-	-	4201				1.03			-3.0	-3.3	-4.6	0.13%	0.05%	0.00%
isotridecan-1-ol	248-469-2	27458-92-0	27458920	-	-	4202	2.69	0.32	3	2.00	0.30		-3.0	-3.3	-4.6	0.13%	0.05%	0.00%
Distillates (coal tar), benzole fraction	283-482-7	84650-02-2	84650022	-	-	4203	4.12	0.38	3	3.12	0.38		-3.0	-3.3	-4.6	0.12%	0.05%	0.00%
Fatty acids, C8-10, Me esters	287-636-4	85566-26-3	85566263	-	-	4204	4.01	0.71	3	3.01	0.71		-3.0	-3.3	-4.6	0.12%	0.05%	0.00%
Resin acids and Rosin acids, esters with pentaerythritol	232-479-9	8050-26-8	8050268	-	-	4205	6.20	0.63	3	5.20	0.63		-3.0	-3.3	-4.6	0.12%	0.05%	0.00%
Distillates (coal tar), light oils	283-483-2	84650-03-3	84650033	-	-	4206	4.04		2				-3.0	-3.3	-4.6	0.12%	0.05%	0.00%
Alcohols, C12-13, branched and linear, ethoxylated, sulfates, sod	500-513-4	161074-79-9	161074799	-	-	4207	4.02	0.43	3	3.02	0.43		-3.0	-3.3	-4.7	0.12%	0.05%	0.00%
Fatty acids, C8-10	273-086-2	68937-75-7	68937757	-	-	4208	3.99	0.66	3	2.99	0.66		-3.0	-3.3	-4.7	0.11%	0.05%	0.00%
Dodecene, branched	306-479-5	97280-83-6	97280836	-	-	4209	2.24	1.03	3	3.94	2.01		-3.1	-3.3	-4.7	0.11%	0.05%	0.00%
Fatty acids, C16-18, zinc salts	293-049-4	91051-01-3	91051013	-	-	4210	3.08	0.69	3	1.89	0.67		-3.1	-3.3	-4.7	0.11%	0.05%	0.00%
1234694-02-0	629-780-6	1234694-02-0	1234694020	-	-	4211	5.74		1	5.00			-3.1	-3.3	-4.7	0.11%	0.05%	0.00%
1,2-Dihydro-2,2,4-trimethylquinoline, oligomers	500-051-3	26780-96-1	26780961	-	-	4212	4.97	0.98	3	3.97	0.98		-3.1	-3.3	-4.7	0.10%	0.04%	0.00%
620-174-7	620-174-7	1079184-43-2	1079184432	-	-	4213	3.82	0.26	3	2.71	0.17		-3.1	-3.3	-4.7	0.10%	0.04%	0.00%
(2-methoxymethylethoxy)propanol	252-104-2	34590-94-8	34590948	-	-	4214	6.71	0.48	3	5.71	0.48		-3.1	-3.3	-4.7	0.10%	0.04%	0.00%
Fatty acids, tall-oil, low-boiling	266-039-2	65997-03-7	65997037	-	-	4215	4.95	0.77	3	3.95	0.77		-3.1	-3.3	-4.7	0.10%	0.04%	0.00%
Sulfonic acids, C14-17-sec-alkane, sodium salts	307-055-2	97489-15-1	97489151	-	-	4216	4.30	0.54	3	3.15	0.73		-3.1	-3.4	-4.7	0.10%	0.04%	0.00%
4,4'-Methylenediphenyl diisocyanate, oligomers	500-040-3	25686-28-6	25686286	-	-	4217	6.37	0.26	3	5.37	0.26		-3.1	-3.4	-4.7	0.09%	0.04%	0.00%
citral	226-394-6	5392-40-5	5392405	-	-	4218	4.65	0.81	5	3.05	0.10		-3.1	-3.4	-4.7	0.09%	0.04%	0.00%
Phenol, dodecyl-, branched	310-154-3	121158-58-5	121158585	-	-	4219	3.50	1.32	3	2.38	1.09		-3.1	-3.4	-4.7	0.09%	0.04%	0.00%
Glycerides, C16-18	268-084-3	68002-71-1	68002711	-	-	4220	5.73	0.72	3	4.73	0.72		-3.1	-3.4	-4.7	0.09%	0.04%	0.00%
Extracts, coal tar oil alk.	266-017-2	65996-83-0	65996830	-	-	4221	4.14		2				-3.1	-3.4	-4.7	0.08%	0.03%	0.00%
Carboxylic acids, di-, C4-6	271-678-5	68603-87-2	68603872	-	-	4222	4.80	0.26	3	4.17	0.33		-3.1	-3.4	-4.7	0.08%	0.03%	0.00%
Phenol, dodecyl-, sulfurized, carbonates, calcium salts, overbase	272-234-3	68784-26-9	68784269	-	-	4223	6.07	0.42	3	5.07	0.42		-3.1	-3.4	-4.8	0.08%	0.03%	0.00%
Rosin, fumarated	266-040-8	65997-04-8	65997048	-	-	4224	4.20	0.28	3	4.18	0.78		-3.2	-3.4	-4.8	0.08%	0.03%	0.00%
Alcohols, C13-15-branched and linear	287-625-4	85566-16-1	85566161	-	-	4225	3.99	1.76	3	3.26	1.33		-3.2	-3.4	-4.8	0.08%	0.03%	0.00%
Anthracene oil, anthracene paste	292-603-2	90640-81-6	90640816	-	-	4226	4.70		2				-3.2	-3.4	-4.8	0.08%	0.03%	0.00%
Resin acids and Rosin acids, esters with glycerol	232-482-5	8050-31-5	8050315	-	-	4227	6.20	0.63	3	5.20	0.63		-3.2	-3.4	-4.8	0.08%	0.03%	0.00%
692-061-0	692-061-0	1207435-39-9	1207435399	-	-	4228	5.25	0.45	3	4.25	0.45		-3.2	-3.4	-4.8	0.08%	0.03%	0.00%
Alcohols, C12-13, branched and linear, ethoxylated	500-457-0	160901-19-9	160901199	-	-	4229	2.79	0.57	3	1.79	0.57		-3.2	-3.4	-4.8	0.08%	0.03%	0.00%
Fatty acids, C16-18 and C18-unsatd., branched and linear	273-295-9	68955-98-6	68955986	-	-	4230	6.14	0.96	3	5.14	0.96		-3.2	-3.4	-4.8	0.07%	0.03%	0.00%
Nonene, branched	306-492-6	97280-95-0	97280950	-	-	4231	3.32	1.28	3	3.84	2.11		-3.2	-3.4	-4.8	0.07%	0.03%	0.00%
Alkenes, C20-24 α-	300-202-1	93924-10-8	93924108	-	-	4232	3.32	1.28	3	3.84	2.11		-3.2	-3.5	-4.8	0.07%	0.03%	0.00%
Formaldehyde, oligomeric reaction products with 1-chloro-2,3-e	500-006-8	9003-36-5	9003365	-	-	4233	4.47	0.93	3	3.47	0.93		-3.2	-3.5	-4.8	0.07%	0.03%	0.00%
Alcohols, C12-13	278-306-0	75782-86-4	75782864	-	-	4234	3.00	0.63	3	2.00	0.63		-3.2	-3.5	-4.8	0.07%	0.03%	0.00%
Fatty acids, C12-18 and C18-unsatd., 2-sulfoethyl esters, sodium	287-024-7	85408-62-4	85408624	-	-	4235	3.25	0.32	3	2.25	0.32		-3.2	-3.5	-4.8	0.07%	0.03%	0.00%
Amines, polyethylenepoly-, triethylenetetramine fraction	292-588-2	90640-67-8	90640678	-	-	4236	4.70	0.76	3	3.70	0.76		-3.2	-3.5	-4.8	0.07%	0.03%	0.00%
Orange, sweet, ext.	232-433-8	8028-48-6	8028486	-	-	4237	4.22	0.75	3	3.54	0.53		-3.2	-3.5	-4.8	0.06%	0.03%	0.00%
Fatty acids, C12-18	266-925-9	67701-01-3	67701013	-	-	4238	4.49	1.59	3	3.49	1.59		-3.2	-3.5	-4.8	0.06%	0.02%	0.00%
Fatty acids, C8-18	292-769-6	90990-08-2	90990082	-	-	4239	4.49	1.59	3	3.49	1.59		-3.2	-3.5	-4.8	0.06%	0.02%	0.00%
hexabromocyclododecane	247-148-4	25637-99-4	25637994	-	-	4240	1.12	0.58	7	0.71	0.57		-3.2	-3.5	-4.8	0.06%	0.02%	0.00%
Methyl dodec-9-enoate	700-618-7	39202-17-0	39202170	-	-	4241	2.71	0.46	3	1.71	0.46		-3.2	-3.5	-4.8	0.06%	0.02%	0.00%
tert-dodecanethiol	246-619-1	25103-58-6	25103586	-	-	4242	3.52	1.80	3	2.52	1.80		-3.2	-3.5	-4.8	0.06%	0.02%	0.00%
Alcohols, C12-15-branched and linear	292-334-0	90604-40-3	90604403	-	-	4243	3.37	0.95	3	2.37	0.95		-3.2	-3.5	-4.8	0.06%	0.02%	0.00%
Resin acids and Rosin acids, sodium salts	263-144-5	61790-51-0	61790510	-	-	4244	4.13	1.14	3	3.79	1.27		-3.2	-3.5	-4.8	0.06%	0.02%	0.00%
ethanol, 2-butoxy-, manufacture of, by-products from	310-287-7	161907-77-3	161907773	-	-	4245	5.80		2				-3.2	-3.5	-4.9	0.06%	0.02%	0.00%
629-695-4	629-695-4	164383-22-6	164383226	-	-	4246	2.91	0.41	3	1.91	0.41		-3.3	-3.5	-4.9	0.06%	0.02%	0.00%
2-Oxetanone, 3-C12-16-alkyl-4-C13-17-alkylidene derivs.	284-932-5	84989-41-3	84989413	-	-	4247	4.92	1.44	3	3.92	1.44		-3.3	-3.5	-4.9	0.05%	0.02%	0.00%
Fatty acids, C16-18, Me esters	287-824-6	85586-21-6	85586216	-	-	4248	5.42	1.74	3	4.42	1.74		-3.3	-3.5	-4.9	0.05%	0.02%	0.00%
2,5-Furandione, dihydro-, mono-C15-20-alkenyl derivs.	272-221-2	68784-12-3	68784123	-	-	4249	4.62	0.31	3	3.62	0.31		-3.3	-3.5	-4.9	0.05%	0.02%	0.00%
Castor oil, hydrogenated	232-292-2	8001-78-3	8001783	-	-	4250	4.83	2.66	3	3.83	2.66		-3.3	-3.5	-4.9	0.05%	0.02%	0.00%
Sugar, invert	232-393-1	8013-17-0	8013170	-	-	4251							-3.3	-3.5	-4.9	0.05%	0.02%	0.00%
Alcohols, C9-11	266-367-6	66455-17-2	66455172	-	-	4252	3.68	0.16	3	2.68	0.16		-3.3	-3.5	-4.9	0.05%	0.02%	0.00%
Fatty acids, essential, Et esters	293-054-1	91051-05-7	91051057	-	-	4253	4.93	1.02	3	3.93	1.02		-3.3	-3.5	-4.9	0.05%	0.02%	0.00%
Resin acids and Rosin acids, fumarated, esters with pentaerythri	305-514-1	94581-15-4	94581154	-	-	4254							-3.3	-3.5	-4.9	0.05%	0.02%	0.00%
Amines, C16-18 and C18-unsatd. alkyl	268-219-6	68037-95-6	68037956	-	-	4255	2.25	0.77	3	1.46	0.71		-3.3	-3.5	-4.9	0.05%	0.02%	0.00%
Alcohols, C11-14-iso-, C13-rich	271-235-6	68526-86-3	68526863	-	-	4256	2.80	0.48	3	2.18	0.45		-3.3	-3.5	-4.9	0.05%	0.02%	0.00%
Octene, hydroformylation products, high-boiling	271-237-7	68526-89-6	68526896	-	-	4257	5.42	0.54	3	4.42	0.54		-3.3	-3.6	-4.9	0.05%	0.02%	0.00%
Octene, hydroformylation products, low-boiling	273-110-1	68938-03-4	68938034	-	-	4258	4.50	0.27	3	3.50	0.27		-3.3	-3.6	-4.9	0.05%	0.02%	0.00%
Glycerides, C8-18 and C18-unsatd.	266-946-3	67701-28-4	67701284	-	-	4259	5.73	0.72	3	4.73	0.72		-3.3	-3.6	-4.9	0.05%	0.02%	0.00%

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Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [·]	Z(Cwfresh) [·]	Z(Cwcoast) [·]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
692-840-5	692-840-5	1345668-40-7	1345668407	-	-	4260	6.54	0.42	3	5.54	0.42		-3.3	-3.6	-4.9	0.05%	0.02%	0.00%
Sulfonic acids, C10-21-alkane, Ph esters	293-728-5	91082-17-6	91082176	-	-	4261	4.65	0.98	3	3.65	0.98		-3.3	-3.6	-4.9	0.05%	0.02%	0.00%
Amines, C16-18-alkyl	292-550-5	90640-32-7	90640327	-	-	4262	2.25	0.78	3	1.48	0.71		-3.3	-3.6	-4.9	0.04%	0.02%	0.00%
Paraffin waxes and Hydrocarbon waxes, chloro	264-150-0	63449-39-8	63449398	-	-	4263	5.61	0.48	7	4.61	0.48		-3.3	-3.6	-4.9	0.04%	0.02%	0.00%
3(or 4)-methylbenzene-1,2-diamine	248-145-0	26966-75-6	26966756	-	-	4264	3.10	1.09	3	1.79	1.17		-3.3	-3.6	-4.9	0.04%	0.02%	0.00%
Paraffin waxes and Hydrocarbon waxes, chloro, sulfochlorinated	269-145-7	68188-19-2	68188192	-	-	4265							-3.4	-3.6	-5.0	0.04%	0.02%	0.00%
Hydrocarbons, C14-30, olefin-rich	271-036-4	68514-35-2	68514352	-	-	4266	6.50		3	5.50			-3.4	-3.6	-5.0	0.04%	0.02%	0.00%
Cyclohexane, oxidized, non-acidic by-products, distn. residues	271-816-4	68609-04-1	68609041	-	-	4267	4.55	0.10	3	3.55	0.10		-3.4	-3.6	-5.0	0.04%	0.02%	0.00%
Cyclohexane, oxidized, aq. ext., sodium salt	272-812-5	68915-39-9	68915399	-	-	4268							-3.4	-3.6	-5.0	0.04%	0.02%	0.00%
Fatty acids, C8-24	275-164-1	71076-48-7	71076487	-	-	4269	4.09	0.96	3	3.58	1.48		-3.4	-3.6	-5.0	0.04%	0.02%	0.00%
Naphtha, thermal cracked, residues, naphthalene cut	285-562-7	85117-10-8	85117108	-	-	4270	3.64	0.51	3	2.97	0.56		-3.4	-3.6	-5.0	0.04%	0.02%	0.00%
Alkenes, C9-13-branched, C10-rich	295-253-9	91994-95-5	91994955	-	-	4271	2.96	0.82	3	3.44	2.00		-3.4	-3.6	-5.0	0.04%	0.02%	0.00%
Alkenes, C7-9-branched, C8-rich	307-300-3	97593-00-5	97593005	-	-	4272	2.96	0.82	3	3.44	2.00		-3.4	-3.6	-5.0	0.04%	0.02%	0.00%
bis(nonylphenyl)amine	253-249-4	36878-20-3	36878203	-	-	4273	4.98	0.28	3	3.98	0.28		-3.4	-3.6	-5.0	0.04%	0.02%	0.00%
Glycerides, C16-18 mono- and di-	286-490-9	85251-77-0	85251770	-	-	4274	4.83	2.66	3	3.83	2.66		-3.4	-3.6	-5.0	0.04%	0.01%	0.00%
Creosote oil	263-047-8	61789-28-4	61789284	-	-	4275	3.68	0.73	6	2.71	1.03		-3.4	-3.6	-5.0	0.04%	0.01%	0.00%
Hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fr	297-629-8	93685-81-5	93685815	-	-	4276	5.37	2.55	3	4.37	2.55		-3.4	-3.6	-5.0	0.04%	0.01%	0.00%
Anthracene oil, anthracene-low	292-604-8	90640-82-7	90640827	-	-	4277	2.88		2				-3.4	-3.6	-5.0	0.03%	0.01%	0.00%
2-Propenoic acid, 2-methyl-, C12-15-branched and linear alkyl es	292-122-8	90552-02-6	90552026	-	-	4278				0.76			-3.4	-3.6	-5.0	0.03%	0.01%	0.00%
Ethylenediamine, propoxylated	500-035-6	25214-63-5	25214635	-	-	4279	5.55	1.18	3	4.55	1.18		-3.4	-3.7	-5.0	0.03%	0.01%	0.00%
1-Propene, chlorinated, epoxidized, distn. residues	304-800-3	94279-54-6	94279546	-	-	4280							-3.4	-3.7	-5.0	0.03%	0.01%	0.00%
Alcohols, C7-9-iso-, C8-rich	271-231-4	68526-83-0	68526830	-	-	4281	4.29	0.13	3	3.29	0.13		-3.4	-3.7	-5.0	0.03%	0.01%	0.00%
nitrotoluene	215-311-9	1321-12-6	1321126	-	-	4282	3.77		1				-3.4	-3.7	-5.0	0.03%	0.01%	0.00%
Distillates (coal tar)	266-027-7	65996-92-1	65996921	-	-	4283	4.70		2				-3.4	-3.7	-5.0	0.03%	0.01%	0.00%
Pitch, coal tar, high-temp., heat-treated	310-162-7	121575-60-8	121575608	-	-	4284	5.83	0.58	3	4.83	0.58		-3.4	-3.7	-5.0	0.03%	0.01%	0.00%
Pentanol, branched and linear	305-536-1	94624-12-1	94624121	-	-	4285	5.73	0.24	3	4.73	0.24		-3.4	-3.7	-5.0	0.03%	0.01%	0.00%
4,4'-Methylenediphenyl diisocyanate, oligomeric reaction produ	500-270-4	88288-99-7	88288997	-	-	4286							-3.4	-3.7	-5.0	0.03%	0.01%	0.00%
627-132-7	627-132-7	1227096-04-9	1227096049	-	-	4287	3.56	1.39	3	2.73	1.34		-3.4	-3.7	-5.0	0.03%	0.01%	0.00%
Poly(oxy-1,2-ethanediyl), α-butyl-ω-hydroxy-	500-012-0	9004-77-7	9004777	-	-	4288	5.76		2				-3.4	-3.7	-5.0	0.03%	0.01%	0.00%
600-975-8	600-975-8	110615-47-9	110615479	-	-	4289	3.89	0.32	3	2.88	0.30		-3.4	-3.7	-5.0	0.03%	0.01%	0.00%
Glycerides, mixed decanoyl and octanoyl	277-452-2	73398-61-5	73398615	-	-	4290	3.46	1.52	3	2.46	1.52		-3.4	-3.7	-5.0	0.03%	0.01%	0.00%
methacrylic acid, monoester with propane-1,2-diol	248-666-3	27813-02-1	27813021	-	-	4291	5.87	0.33	3	4.87	0.33		-3.5	-3.7	-5.1	0.03%	0.01%	0.00%
D-Glucopyranose, oligomers, decyl octyl glycosides	500-220-1	68515-73-1	68515731	-	-	4292	4.77	0.53	3	4.01	0.55		-3.5	-3.7	-5.1	0.03%	0.01%	0.00%
Tar acids, coal, crude	266-019-3	65996-85-2	65996852	-	-	4293	4.22	0.57	3	3.22	0.57		-3.5	-3.7	-5.1	0.03%	0.01%	0.00%
Sulfuric acid, mono-C12-18-alkyl esters, sodium salts	273-257-1	68955-19-1	68955191	-	-	4294	4.01	0.44	3	3.16	0.33		-3.5	-3.7	-5.1	0.03%	0.01%	0.00%
1,2-Benzenedicarboxylic acid, benzyl C7-9-branched and linear a	271-082-5	68515-40-2	68515402	-	-	4295	2.87		1	1.59			-3.5	-3.7	-5.1	0.03%	0.01%	0.00%
4,4'-Isopropylidenediphenol, oligomeric reaction products with 1	500-130-2	55818-57-0	55818570	-	-	4296	4.36		1				-3.5	-3.7	-5.1	0.03%	0.01%	0.00%
Phenol, isopropylated	291-826-2	90480-88-9	90480889	-	-	4297							-3.5	-3.7	-5.1	0.03%	0.01%	0.00%
614-144-2	614-144-2	67800-94-6	67800946	-	-	4298	5.37	0.26	3	4.37	0.26		-3.5	-3.7	-5.1	0.03%	0.01%	0.00%
Fatty acids, C16-18, esters with ethylene glycol	292-932-1	91031-31-1	91031311	-	-	4299							-3.5	-3.7	-5.1	0.02%	0.01%	0.00%
Fatty acids, tall-oil, reaction products with diethylenetriamine, m	273-601-0	68990-47-6	68990476	-	-	4300							-3.5	-3.7	-5.1	0.02%	0.01%	0.00%
Amines, polyethylenepoly-	268-626-9	68131-73-7	68131737	-	-	4301	3.62	1.17	3	2.62	1.17		-3.5	-3.7	-5.1	0.02%	0.01%	0.00%
Propylidynetrimethanol, propoxylated	500-041-9	25723-16-4	25723164	-	-	4302	5.64	0.61	3	4.71	0.53		-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
Amines, C20-22-alkyldimethyl	296-866-4	93164-85-3	93164853	-	-	4303	2.17	2.15	3	1.17	2.15		-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
Amines, polyethylenepoly-, tetraethylenepentamine fraction	292-587-7	90640-66-7	90640667	-	-	4304	4.53	0.99	3	3.53	0.99		-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
pentene	246-916-6	25377-72-4	25377724	-	-	4305	4.51	0.74	3	3.51	0.74		-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethyl	270-128-1	68411-46-1	68411461	-	-	4306	4.98	0.28	3	3.98	0.28		-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
Fatty acids, C14-18 and C16-18 unsatd., triesters with trimethylo	268-093-2	68002-79-9	68002799	-	-	4307	6.74		1	5.04			-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
Hydrocarbons, C5-rich, dicyclopentadiene-contg.	310-013-6	102110-15-6	102110156	-	-	4308	3.36	0.52	3	2.79	1.10		-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
Tar acids, brown-coal gasification	295-536-7	92062-22-1	92062221	-	-	4309	4.22	0.57	3	3.22	0.57		-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
Oils, vegetable, deodorizer distillates	270-700-0	68476-80-2	68476802	-	-	4310	4.36		2				-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
Glycerides, C16-18 mono-	293-208-8	91052-47-0	91052470	-	-	4311	4.83	2.66	3	3.83	2.66		-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
Oils, fish, oxidized, bisulfited, sodium salts	307-037-4	97488-98-7	97488987	-	-	4312	5.35	0.53	3	4.35	0.53		-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
2,2'-Iminodiethanol, propoxylated	500-085-9	35176-06-8	35176068	-	-	4313				4.00			-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
Resin acids and Rosin acids, potassium salts	263-142-4	61790-50-9	61790509	-	-	4314	4.13	1.14	3	3.79	1.27		-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
Acetic acid, oxo-, sodium salt, reaction products with ethylenedi	283-044-5	84539-55-9	84539559	-	-	4315	5.34	0.73	4	4.34	0.73		-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
Glycerol, propoxylated, esters with acrylic acid	500-114-5	52408-84-1	52408841	-	-	4316	4.27	0.62	3	3.27	0.62		-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
Fatty acids, C18-unsatd.	289-450-9	88895-93-6	88895936	-	-	4317							-3.5	-3.8	-5.1	0.02%	0.01%	0.00%
Resin acids and Rosin acids, calcium salts	232-694-8	9007-13-0	9007130	-	-	4318	4.13	1.14	3	3.79	1.27		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
Phenol, isopropylated, phosphate (3:1)	273-066-3	68937-41-7	68937417	-	-	4319	3.96	1.19	3	2.96	1.19		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
Ethane- 1,2-diol, propoxylated	500-078-0	31923-84-9	31923849	-	-	4320				4.00			-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
Oxirane, reaction products with ammonia, distn. residues	273-224-1	68953-70-8	68953708	-	-	4321	6.14	0.73	3	5.14	0.73		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [·]	Z(Cwfresh) [·]	Z(Cwcoast) [·]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Fatty acids, C16-18, esters with pentaerythritol	285-547-5	85116-93-4	85116934	-	-	4322	5.74	0.97	3	4.74	0.97		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
Extract residues (coal), light oil alk., acid ext., indene fraction	309-867-2	101316-62-5	101316625	-	-	4323	3.36	0.52	3	2.79	1.10		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
Propylidynetrimethanol, ethoxylated, esters with acrylic acid	500-066-5	28961-43-5	28961435	-	-	4324	3.83	0.89	3	2.83	0.89		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
1,4-Benzenedicarboxylic acid, dimethyl ester, manuf. of, by-prod	273-521-6	68988-22-7	68988227	-	-	4325	4.23	0.74	3	3.23	0.74		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
Montan wax	232-313-5	8002-53-7	8002537	-	-	4326							-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
isooctadecanoic acid	250-178-0	30399-84-9	30399849	-	-	4327	6.03	1.10	3	5.03	1.10		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
Polysulfides, di-tert-Bu	273-103-3	68937-96-2	68937962	-	-	4328	3.36	0.68	3	2.36	0.68		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
Solvent naphtha (coal), xylene-styrene cut	287-502-5	85536-20-5	85536205	-	-	4329	3.62	0.26	3	2.62	0.26		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
1,2,4-Benzenetricarboxylic acid, mixed decyl and octyl triesters	290-754-9	90218-76-1	90218761	-	-	4330	4.14	0.31	3	3.14	0.31		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
603-309-4	603-309-4	128973-77-3	128973773	-	-	4331	3.05		2	1.94			-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
Amines, C12-18-alkyl	268-953-7	68155-27-1	68155271	-	-	4332	2.25	0.78	3	1.48	0.71		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
Resin acids and Rosin acids, magnesium salts	270-461-2	68440-56-2	68440562	-	-	4333	4.13	1.14	3	3.79	1.27		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
619-079-3	619-079-3	949109-75-5	949109755	-	-	4334							-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
orthoboric acid, compound with 2-aminoethanol	247-421-8	26038-87-9	26038879	-	-	4335	5.08	0.51	3	4.08	0.51		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
Fatty acids, C14-18 and C16-18-unsatd., zinc salts	266-936-9	67701-12-6	67701126	-	-	4336	3.16	0.72	3	1.89	0.67		-3.6	-3.8	-5.2	0.02%	0.01%	0.00%
Glycerides, tall-oil mono-, di-, and tri-	307-751-6	97722-02-6	97722026	-	-	4337	4.83	2.66	3	3.83	2.66		-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
Dodecene, hydroformylation products, low-boiling	271-240-3	68526-92-1	68526921	-	-	4338	3.83		1				-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
tetrahydromethylphthalic anhydride	234-290-7	11070-44-3	11070443	-	-	4339	5.00	0.17	3	4.33	0.23		-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
Saccharomyces cerevisiae, ext.	283-294-5	84604-16-0	84604160	-	-	4340							-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
Benzene, (1-methylethyl)-, oxidized, cumene residues, acetophe	309-849-4	101316-44-3	101316443	-	-	4341	4.69		2				-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
Distillates (petroleum), heavy steam-cracked	309-939-3	101631-14-5	101631145	-	-	4342	3.63	0.51	3	3.01	0.57		-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
2,6-dimethylmorpholine	205-509-3	141-91-3	141913	-	-	4343	5.39	0.19	4	4.45	0.16		-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
Glycerides, C14-18	266-945-8	67701-27-3	67701273	-	-	4344	4.83	2.66	3	3.83	2.66		-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
Hydrocarbons, C4-10-unsatd.	271-040-6	68514-38-5	68514385	-	-	4345	2.96	0.82	3	3.44	2.00		-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
Alkenes, C6-	271-208-9	68526-52-3	68526523	-	-	4346	3.69	0.33	3	2.69	0.33		-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
Alkenes, C10-12, C11-rich	271-214-1	68526-57-8	68526578	-	-	4347	2.96	0.82	3	3.44	2.00		-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
Alkenes, C6-10, hydroformylation products, high-boiling	271-230-9	68526-82-9	68526829	-	-	4348							-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
1-Propene, hydroformylation products, high-boiling	271-363-2	68551-11-1	68551111	-	-	4349	5.04	0.24	3	4.03	0.16		-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
Hydrocarbons, C4 and C8, butene concentrator by-product	271-739-6	68606-29-1	68606291	-	-	4350	1.72	0.19	3	0.72	0.19		-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
Disilane, chloro Me derivs.	273-054-8	68937-17-7	68937177	-	-	4351	5.44	0.82	3	4.44	0.82		-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
1,2-Benzenedicarboxylic acid, di-C1-13 alkyl esters, manuf. of, by	284-310-3	84852-02-8	84852028	-	-	4352	3.64		2				-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
Alkyl iodides, C8-14, γ-ω-perfluoro	289-100-5	85995-91-1	85995911	-	-	4353							-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
Naphtha (coal), distn. residues	292-636-2	90641-12-6	90641126	-	-	4354	4.87	0.89	3	3.87	0.89		-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
anthracene oil, anthracene paste, distn. lights	295-278-5	91995-17-4	91995174	-	-	4355	4.70		2				-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
Alkenes, C11-14	297-794-6	93762-77-7	93762777	-	-	4356	4.50	2.82	3	3.50	2.82		-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
Alkenes, C6-8-branched, C7-rich	307-298-4	97592-99-9	97592999	-	-	4357	2.96	0.82	3	3.44	2.00		-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
bis(isopropyl)naphthalene	254-052-6	38640-62-9	38640629	-	-	4358	3.89	0.66	3	2.34	0.70		-3.6	-3.9	-5.2	0.02%	0.01%	0.00%
Propylidynetrimethanol, ethoxylated	500-110-3	50586-59-9	50586599	-	-	4359	5.83	1.00	3	4.83	1.00		-3.6	-3.9	-5.2	0.01%	0.01%	0.00%
Terpineol	232-268-1	8000-41-7	8000417	-	-	4360	4.75	0.23	3	3.75	0.23		-3.6	-3.9	-5.2	0.01%	0.01%	0.00%
oxydipropyl dibenzoate	248-258-5	27138-31-4	27138314	-	-	4361	3.65	0.68	3	2.42	0.51		-3.6	-3.9	-5.2	0.01%	0.01%	0.00%
Paraffin oils, sulfochlorinated, saponified	269-144-1	68188-18-1	68188181	-	-	4362	3.82	0.99	3	2.63	0.79		-3.6	-3.9	-5.2	0.01%	0.01%	0.00%
601-601-6	601-601-6	119345-04-9	119345049	-	-	4363	4.45	1.01	3	3.45	1.01		-3.6	-3.9	-5.2	0.01%	0.01%	0.00%
603-094-7	603-094-7	125904-11-2	125904112	-	-	4364	3.66	0.25	3	2.45	0.44		-3.6	-3.9	-5.2	0.01%	0.01%	0.00%
methyl 3-oxo-2-pentylcyclopentaneacetate	246-495-9	24851-98-7	24851987	-	-	4365	4.30	0.24	3	3.06	0.38		-3.6	-3.9	-5.2	0.01%	0.01%	0.00%
4,4'-methylenebis(cyclohexylamine)	217-168-8	1761-71-3	1761713	-	-	4366	4.88	0.82	3	4.03	0.84		-3.6	-3.9	-5.2	0.01%	0.01%	0.00%
diisononyl adipate	251-646-7	33703-08-1	33703081	-	-	4367				2.89			-3.6	-3.9	-5.2	0.01%	0.01%	0.00%
Rosin, reaction products with formaldehyde	293-659-0	91081-53-7	91081537	-	-	4368	4.13	1.14	3	3.79	1.27		-3.6	-3.9	-5.2	0.01%	0.01%	0.00%
ditolyl ether	248-948-6	28299-41-4	28299414	-	-	4369	2.37	0.80	3	1.37	0.80		-3.6	-3.9	-5.2	0.01%	0.00%	0.00%
627-034-4	627-034-4	1213789-63-9	1213789639	-	-	4370	2.25	0.78	3	1.48	0.71		-3.6	-3.9	-5.2	0.01%	0.00%	0.00%
Amides, coco, N-[3-(dimethylamino)propyl]	268-771-8	68140-01-2	68140012	-	-	4371	2.60		1				-3.6	-3.9	-5.2	0.01%	0.00%	0.00%
Linseed oil, oxidized	272-038-8	68649-95-6	68649956	-	-	4372	4.79		2				-3.6	-3.9	-5.2	0.01%	0.00%	0.00%
Fatty acids, C5-10, esters with pentaerythritol	270-291-9	68424-31-7	68424317	-	-	4373	5.55	0.91	3	4.55	0.91		-3.6	-3.9	-5.3	0.01%	0.00%	0.00%
Phenol, 4-methyl-, reaction products with dicyclopentadiene an	271-867-2	68610-51-5	68610515	-	-	4374							-3.7	-3.9	-5.3	0.01%	0.00%	0.00%
hexadecene	248-131-4	26952-14-7	26952147	-	-	4375	3.32	1.28	3	3.84	2.11		-3.7	-3.9	-5.3	0.01%	0.00%	0.00%
2,2'-Oxydiethanol, propoxylated	500-031-4	9051-51-8	9051518	-	-	4376				4.00			-3.7	-3.9	-5.3	0.01%	0.00%	0.00%
Benzenesulfonic acid, mono-C10-13-alkyl derivs., compds. with a	287-335-8	85480-55-3	85480553	-	-	4377	3.84	0.61	4	3.15	0.55		-3.7	-3.9	-5.3	0.01%	0.00%	0.00%
Fatty acids, C16-18, C16-18-alkyl esters	306-797-4	97404-33-6	97404336	-	-	4378	5.00		1				-3.7	-3.9	-5.3	0.01%	0.00%	0.00%
1,6-bis(2,3-epoxypropoxy)hexane	240-260-4	16096-31-4	16096314	-	-	4379	4.49	0.15	3	3.49	0.15		-3.7	-3.9	-5.3	0.01%	0.00%	0.00%
Alcohols, C9-11-branched	271-360-6	68551-08-6	68551086	-	-	4380	3.13	0.41	3	2.13	0.41		-3.7	-3.9	-5.3	0.01%	0.00%	0.00%
Rosin, hydrogenated	266-041-3	65997-06-0	65997060	-	-	4381	4.52	0.81	3	3.89	1.10		-3.7	-3.9	-5.3	0.01%	0.00%	0.00%
Protein hydrolyzates, animal	309-203-1	100085-61-8	100085618	-	-	4382							-3.7	-3.9	-5.3	0.01%	0.00%	0.00%
Dec-1-ene, dimers, hydrogenated	500-228-5	68649-11-6	68649116	-	-	4383	6.46	0.14	3	5.46	0.14		-3.7	-3.9	-5.3	0.01%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
4,4'-Methylenediphenyl diisocyanate, oligomeric reaction produ	500-262-0	75880-28-3	75880283	-	-	4384	6.42	1.23	3	5.42	1.23		-3.7	-3.9	-5.3	0.01%	0.00%	0.00%
642-362-8	642-362-8	1190630-03-5	1190630035	-	-	4385							-3.7	-3.9	-5.3	0.01%	0.00%	0.00%
diundecyl phthalate, branched and linear	287-401-6	85507-79-5	85507795	-	-	4386	3.72	0.67	3	2.72	0.67		-3.7	-3.9	-5.3	0.01%	0.00%	0.00%
oxybis(methyl-2,1-ethanediyl) diacrylate	260-754-3	57472-68-1	57472681	-	-	4387	4.03	0.46	3	2.78	0.25		-3.7	-4.0	-5.3	0.01%	0.00%	0.00%
diisotridecyl adipate	247-660-8	26401-35-4	26401354	-	-	4388	5.71		2	1.32			-3.7	-4.0	-5.3	0.01%	0.00%	0.00%
polychloro copper phthalocyanine	215-524-7	1328-53-6	1328536	-	-	4389	5.40		2	3.00			-3.7	-4.0	-5.3	0.01%	0.00%	0.00%
Benzene, (1-methylethyl)-, distn. residues	273-050-6	68936-98-1	68936981	-	-	4390	3.55		2				-3.7	-4.0	-5.3	0.01%	0.00%	0.00%
1,2-Benzenedicarboxylic acid, di-C16-18-alkyl esters	290-580-3	90193-76-3	90193763	-	-	4391							-3.7	-4.0	-5.3	0.01%	0.00%	0.00%
Resin acids and Rosin acids, esters with triethylene glycol	232-478-3	8050-25-7	8050257	-	-	4392	6.20	0.63	3	5.20	0.63		-3.7	-4.0	-5.3	0.01%	0.00%	0.00%
1,2-Benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C	271-089-3	68515-47-9	68515479	-	-	4393	3.17	0.52	3	2.53	0.55		-3.7	-4.0	-5.3	0.01%	0.00%	0.00%
628-856-6	628-856-6	1218787-29-1	1218787291	-	-	4394	2.87	1.27	3	1.61	0.78		-3.7	-4.0	-5.3	0.01%	0.00%	0.00%
Decanoic acid, ester with 2-ethyl-2-(hydroxymethyl)-1,3-propane	234-392-1	11138-60-6	11138606	-	-	4395	4.99		1	6.41			-3.7	-4.0	-5.3	0.01%	0.00%	0.00%
Alcohols, C6-24, distn. residues	310-080-1	102242-49-9	102242499	-	-	4396	6.83	1.15	3	5.83	1.15		-3.7	-4.0	-5.3	0.01%	0.00%	0.00%
604-767-8	604-767-8	151006-60-9	151006609	-	-	4397	6.46	0.14	3	5.46	0.14		-3.7	-4.0	-5.3	0.01%	0.00%	0.00%
Fatty acids, C16-18 and C18-unsatd., Me esters, distn. residues	271-692-1	68604-41-1	68604411	-	-	4398	5.83	1.53	3	4.83	1.53		-3.7	-4.0	-5.3	0.01%	0.00%	0.00%
Phosphorodithioic acid, mixed O,O-bis(1,3-dimethylbutyl and iso	283-392-8	84605-29-8	84605298	-	-	4399	4.29	0.37	3	3.29	0.37		-3.7	-4.0	-5.3	0.01%	0.00%	0.00%
dibenzyltoluene	248-097-0	26898-17-9	26898179	-	-	4400	2.09	1.00	3	1.09	1.00		-3.7	-4.0	-5.3	0.01%	0.00%	0.00%
Phosphorodithioic acid, mixed O,O-bis(sec-Bu and 1,3-dimethylb	272-238-5	68784-31-6	68784316	-	-	4401	4.84	0.77	3	3.84	0.77		-3.7	-4.0	-5.3	0.01%	0.00%	0.00%
Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu a	288-917-4	85940-28-9	85940289	-	-	4402	3.57	0.20	3	2.59	0.13		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
Oils, fish, oxidized	269-122-1	68187-75-7	68187757	-	-	4403							-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
Oxirane, mono[(C12-14-alkyloxy)methyl] derivs.	271-846-8	68609-97-2	68609972	-	-	4404	5.77	1.49	3	4.77	1.49		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
diundecyl phthalate	222-884-9	3648-20-2	3648202	-	-	4405	3.03	0.74	8	2.42	0.67		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
isooctyl acrylate	249-707-8	29590-42-9	29590429	-	-	4406	2.81	0.24	3	1.81	0.24		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylindeno[5,6-c]pyran	214-946-9	1222-05-5	1222055	-	-	4407	2.93	0.19	3	1.93	0.19		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
Fatty acids, hydrogenated tallow, distn. residues	274-307-5	70084-85-4	70084854	-	-	4408							-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
ethanol, 2-methoxy-, manufacture of, by-products from	310-289-8	161907-79-5	161907795	-	-	4409	7.45	0.61	3	6.25	0.65		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
Heptanoic acid, mixed esters with pentaerythritol and valeric aci	270-474-3	68441-94-1	68441941	-	-	4410	5.13	0.96	3	4.13	0.96		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
Fatty acids, tall-oil, oligomeric reaction products with maleic anh	500-451-8	160901-14-4	160901144	-	-	4411	5.50		3	4.50			-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
Cashew, nutshell liq.	232-355-4	8007-24-7	8007247	-	-	4412	5.75	0.98	3	4.75	0.98		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
zinc bis[O,O-bis(2-ethylhexyl)] bis(dithiophosphate)	224-235-5	4259-15-8	4259158	-	-	4413	4.84	0.77	3	3.84	0.77		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
Quaternary ammonium compounds, di-C16-18-alkyldimethyl, ch	295-835-2	92129-33-4	92129334	-	-	4414	2.88	0.87	3	2.17	0.44		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
Alcohols, C16-18 and C18-unsatd., ethoxylated	500-236-9	68920-66-1	68920661	-	-	4415	3.42	0.73	3	2.42	0.73		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
Oils, vegetable, sulfonated, sodium salts	307-044-2	97489-04-8	97489048	-	-	4416	5.35	0.53	3	4.35	0.53		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
DL-menthol	216-074-4	1490-04-6	1490046	-	-	4417	4.36	0.18	3	3.77	0.73		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
Alkanes, C16-20-iso-	292-461-1	90622-59-6	90622596	-	-	4418	2.04	0.30	3	1.04	0.30		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
Extract residues (coal), naphthalene oil alk., distn. residues	292-628-9	90641-05-7	90641057	-	-	4419	4.01	0.88	3	3.01	1.11		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
Extract residues (coal), benzole fraction acid	298-725-2	93821-38-6	93821386	-	-	4420	3.53		1				-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
Humic acids, potassium salts	271-030-1	68514-28-3	68514283	-	-	4421	5.47	0.22	3	4.47	0.22		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
octadecene	248-205-6	27070-58-2	27070582	-	-	4422	3.32	1.28	3	3.84	2.11		-3.8	-4.0	-5.4	0.01%	0.00%	0.00%
xylenesulphonic acid	246-839-8	25321-41-9	25321419	-	-	4423	5.62		2				-3.8	-4.1	-5.4	0.01%	0.00%	0.00%
1,2-Benzenedicarboxylic acid, di-C9-11-branched and linear alkyl	271-085-1	68515-43-5	68515435	-	-	4424	4.10	1.49	3	3.10	1.49		-3.8	-4.1	-5.4	0.01%	0.00%	0.00%
Fatty acids, C16-18 and C18-unsatd., 2-ethylhexyl esters	285-207-6	85049-37-2	85049372	-	-	4425	6.35	1.10	3	5.35	1.10		-3.8	-4.1	-5.4	0.01%	0.00%	0.00%
Sulfuric acid, mono-C12-16-alkyl esters, sodium salts	277-362-3	73296-89-6	73296896	-	-	4426	3.89	0.41	3	3.10	0.38		-3.8	-4.1	-5.4	0.01%	0.00%	0.00%
615-276-3	615-276-3	71302-83-5	71302835	-	-	4427							-3.8	-4.1	-5.4	0.01%	0.00%	0.00%
potassium methylsilanetriolate	250-807-9	31795-24-1	31795241	-	-	4428	7.26	0.77	3	4.17	0.91		-3.8	-4.1	-5.4	0.01%	0.00%	0.00%
Resin acids and Rosin acids, hydrogenated, esters with glycerol	266-042-9	65997-13-9	65997139	-	-	4429	6.20	0.63	3	5.20	0.63		-3.8	-4.1	-5.4	0.01%	0.00%	0.00%
Distillates (coal tar), naphthalene oil crystn. mother liquor	295-310-8	91995-49-2	91995492	-	-	4430	4.87	0.89	3	3.87	0.89		-3.8	-4.1	-5.4	0.01%	0.00%	0.00%
Alkenes, C7-9, hydroformylation products, distn. residues, heavy	308-482-7	98072-31-2	98072312	-	-	4431							-3.8	-4.1	-5.4	0.01%	0.00%	0.00%
Alcohols, C9-11-branched and linear	288-284-4	85711-26-8	85711268	-	-	4432	3.68	0.16	3	2.68	0.16		-3.8	-4.1	-5.4	0.01%	0.00%	0.00%
Fatty acids, C16-18, 2-ethylhexyl esters	292-951-5	91031-48-0	91031480	-	-	4433	6.35	0.97	3	5.35	0.97		-3.8	-4.1	-5.4	0.01%	0.00%	0.00%
tetraphenyl m-phenylene bis(phosphate)	260-830-6	57583-54-7	57583547	-	-	4434	4.89	0.59	3	3.89	0.59		-3.8	-4.1	-5.4	0.01%	0.00%	0.00%
1-Hexanol, 2-ethyl-, manuf. of, by-products from, distn. residues	271-832-1	68609-68-7	68609687	-	-	4435	4.85	0.25	3	3.85	0.25		-3.8	-4.1	-5.4	0.01%	0.00%	0.00%
Tar acids, methylphenol fraction	284-892-9	84989-04-8	84989048	-	-	4436	4.05	0.22	3	3.46	0.43		-3.8	-4.1	-5.4	0.01%	0.00%	0.00%
629-715-1	629-715-1	1226892-43-8	1226892438	-	-	4437	2.79	0.55	3	1.79	0.55		-3.8	-4.1	-5.4	0.01%	0.00%	0.00%
2,2'-dimethyl-4,4'-methylenebis(cyclohexylamine)	229-962-1	6864-37-5	6864375	-	-	4438	4.00	0.48	3	3.10	0.83		-3.9	-4.1	-5.5	0.01%	0.00%	0.00%
Fatty acids, C8-16	287-973-7	85631-26-1	85631261	-	-	4439	4.46	1.35	3	3.42	0.99		-3.9	-4.1	-5.5	0.01%	0.00%	0.00%
Ethanol, 2-amino-, reaction products with ammonia, by-product	272-729-4	68910-05-4	68910054	-	-	4440	3.94	2.08	3	2.94	2.08		-3.9	-4.1	-5.5	0.01%	0.00%	0.00%
629-721-4	629-721-4	308062-60-4	308062604	-	-	4441	3.18	1.97	3	2.18	1.97		-3.9	-4.1	-5.5	0.01%	0.00%	0.00%
1,4-Benzenediamine, N,N'-mixed Ph and tolyl derivs.	273-227-8	68953-84-4	68953844	-	-	4442	2.51	0.59	3	1.51	0.59		-3.9	-4.1	-5.5	0.01%	0.00%	0.00%
Reaction mass of 6-O-alfa-D-glucopyranosyl-D-fructofuranose ar	700-515-7	1236007-63-8	1236007638	-	-	4443	8.34		1	8.40			-3.9	-4.1	-5.5	0.01%	0.00%	0.00%
Benzoic acid, C12-15-alkyl esters	270-112-4	68411-27-8	68411278	-	-	4444							-3.9	-4.1	-5.5	0.01%	0.00%	0.00%
sodium xylenesulphonate	215-090-9	1300-72-7	1300727	-	-	4445	5.50	0.70	3	4.50	0.70		-3.9	-4.1	-5.5	0.01%	0.00%	0.00%

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Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [·]	Z(Cwfresh) [·]	Z(Cwcoast) [·]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
terphenyl	247-477-3	26140-60-3	26140603	-	-	4446	2.63	0.94	3	1.70	1.24		-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
cresol	215-293-2	1319-77-3	1319773	-	-	4447	4.26	0.84	36	3.46	0.43		-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
Terphenyl, hydrogenated	262-967-7	61788-32-7	61788327	-	-	4448	3.22	1.05	3	2.22	1.05		-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
1,4-bis(2,3-epoxypropoxy)butane	219-371-7	2425-79-8	2425798	-	-	4449	4.82	0.26	3	4.02	0.26		-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
dichloromethylbenzene	249-854-8	29797-40-8	29797408	-	-	4450	2.93	1.55	3	1.93	1.55		-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
617-779-3	617-779-3	85940-94-9	85940949	-	-	4451	5.15		1				-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
Glycerides, C12-18	266-944-2	67701-26-2	67701262	-	-	4452	4.83	2.66	3	3.83	2.66		-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
629-719-3	629-719-3	1219010-04-4	1219010044	-	-	4453	1.85	0.49	3	0.85	0.49		-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
Fatty acids, C5-9, esters with pentaerythritol	270-290-3	68424-30-6	68424306	-	-	4454	5.14	0.94	3	4.14	0.94		-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
601-238-3	601-238-3	113163-37-4	113163374	-	-	4455							-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
4,4'-Methylenediphenyl diisocyanate, oligomeric reaction produ	500-312-1	123714-19-2	123714192	-	-	4456	6.37	0.26	3	5.37	0.26		-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
acrylic acid, monoester with propane-1,2-diol	247-118-0	25584-83-2	25584832	-	-	4457	3.91	0.29	3	3.02	0.51		-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
604-580-1	604-580-1	147256-33-5	147256335	-	-	4458	6.33	0.74	3	5.33	0.74		-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
Dodecene, hydroformylation products, high-boiling	271-239-8	68526-91-0	68526910	-	-	4459	4.96	0.93	3	3.96	0.93		-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
Glycerides, C16-18 and C18-unsatd., deodorizer distillates	272-911-3	68920-03-6	68920036	-	-	4460	5.00		1				-3.9	-4.2	-5.5	0.00%	0.00%	0.00%
Fatty acids, C16-18, sodium salts	270-299-2	68424-38-4	68424384	-	-	4461	4.72	0.50	3	3.93	0.56		-3.9	-4.2	-5.6	0.00%	0.00%	0.00%
Glycerides, C16-18 and C18-unsatd. mono-	294-571-5	91744-09-1	91744091	-	-	4462	5.83	1.25	3	4.83	1.25		-4.0	-4.2	-5.6	0.00%	0.00%	0.00%
Pentaerythritol, propoxylated	500-030-9	9051-49-4	9051494	-	-	4463	5.42	0.25	3	4.42	0.25		-4.0	-4.2	-5.6	0.00%	0.00%	0.00%
Glycerides, C16-18 and C18-unsatd. mono-, di and tri-	294-582-5	91744-20-6	91744206	-	-	4464	4.83	2.66	3	3.83	2.66		-4.0	-4.2	-5.6	0.00%	0.00%	0.00%
Subtilisin	232-752-2	9014-01-1	9014011	-	-	4465	3.39	0.84	3	2.60	1.01		-4.0	-4.2	-5.6	0.00%	0.00%	0.00%
stearic acid, monoester with glycerol	250-705-4	31566-31-1	31566311	-	-	4466	4.83	2.66	3	3.83	2.66		-4.0	-4.2	-5.6	0.00%	0.00%	0.00%
Quaternary ammonium compounds, C20-22-alkyltrimethyl, chlo	271-756-9	68607-24-9	68607249	-	-	4467	3.21	0.56	3	2.21	0.56		-4.0	-4.2	-5.6	0.00%	0.00%	0.00%
diethylmethylbenzenediamine	270-877-4	68479-98-1	68479981	-	-	4468	4.11	1.20	3	3.63	1.09		-4.0	-4.2	-5.6	0.00%	0.00%	0.00%
Polysulfides, di-tert-dodecyl	270-335-7	68425-15-0	68425150	-	-	4469	4.16	1.57	3	3.16	1.57		-4.0	-4.2	-5.6	0.00%	0.00%	0.00%
Fatty acids, coco, 2-ethylhexyl esters	295-366-3	92044-87-6	92044876	-	-	4470	4.91	1.67	3	3.91	1.67		-4.0	-4.2	-5.6	0.00%	0.00%	0.00%
2,2',2''-Nitrilotriethanol, propoxylated	500-094-8	37208-53-0	37208530	-	-	4471	5.42	0.25	3	4.42	0.25		-4.0	-4.2	-5.6	0.00%	0.00%	0.00%
diethylbenzene	246-874-9	25340-17-4	25340174	-	-	4472	3.43	0.62	3	2.10	0.39		-4.0	-4.2	-5.6	0.00%	0.00%	0.00%
Distillates (coal tar), benzole fraction, BTX-rich	309-984-9	101896-26-8	101896268	-	-	4473	4.05	0.39	3	3.05	0.39		-4.0	-4.2	-5.6	0.00%	0.00%	0.00%
Solvent naphtha (coal)	266-013-0	65996-79-4	65996794	-	-	4474	3.36	0.52	3	2.79	1.10		-4.0	-4.2	-5.6	0.00%	0.00%	0.00%
1,3,5-triazine-2,4,6-triamine phosphate	255-449-7	41583-09-9	41583099	-	-	4475	5.99	0.77	3	4.99	0.77		-4.0	-4.2	-5.6	0.00%	0.00%	0.00%
Fatty acids, C14-22, 2-ethylhexyl esters, epoxidized	305-962-8	95370-96-0	95370960	-	-	4476							-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
Rape oil, oxidized	305-871-3	95193-59-2	95193592	-	-	4477	5.22	0.64	3	4.22	0.64		-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
4,4'-Isopropylidenediphenol, propoxylated	500-097-4	37353-75-6	37353756	-	-	4478	4.14	0.33	3	3.14	0.33		-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
Alcohols, lanolin	232-430-1	8027-33-6	8027336	-	-	4479	3.60	1.42	3	2.60	1.42		-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
phenol, 2,4-dinitro-, sulfurized, leuco derivatives	266-273-5	66241-11-0	66241110	-	-	4480	4.95	0.90	3	3.95	0.90		-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
Fatty acids, lanolin	270-302-7	68424-43-1	68424431	-	-	4481	5.50		3	4.50			-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
benzyltoluene	248-654-8	27776-01-8	27776018	-	-	4482	2.73	0.49	3	1.88	0.78		-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
614-503-3	614-503-3	68441-62-3	68441623	-	-	4483	5.73		2				-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
2,2,4(or 2,4,4)-trimethylhexane-1,6-diamine	247-063-2	25513-64-8	25513648	-	-	4484	4.74	0.44	3	4.07	0.48		-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
Fatty acids, C16-18 and C18-unsatd., Bu esters	284-863-0	84988-74-9	84988749	-	-	4485	6.16	1.15	3	5.16	1.15		-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
Fatty acids, C18-unsatd., dimers, 2-ethylhexyl esters	500-204-4	68334-05-4	68334054	-	-	4486	5.27	0.39	3	4.27	0.39		-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
Rosin, fumarated, reaction products with glycerol and pentaeryt	296-047-1	92202-14-7	92202147	-	-	4487							-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
Aromatic hydrocarbons, C9-12, benzene distn.	295-551-9	92062-36-7	92062367	-	-	4488	3.70	0.48	3	2.70	0.48		-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
3,6,9,12-tetraazatetradecamethylenediamine	223-775-9	4067-16-7	4067167	-	-	4489	4.10	0.94	3	3.47	1.55		-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
potassium trihydrogen dioxalate	204-874-6	127-96-8	127968	-	-	4490	5.73	0.56	3	4.73	0.56		-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
Lecithins, acetylated	293-316-5	91053-50-8	91053508	-	-	4491	3.97		1				-4.0	-4.3	-5.6	0.00%	0.00%	0.00%
4,4'-Methylenediphenyl diisocyanate, oligomeric reaction produ	500-415-1	158885-29-1	158885291	-	-	4492	6.37	0.24	3	5.37	0.24		-4.0	-4.3	-5.7	0.00%	0.00%	0.00%
2-aminoethanol, monoester with boric acid	233-829-3	10377-81-8	10377818	-	-	4493	5.08	0.51	3	4.08	0.51		-4.0	-4.3	-5.7	0.00%	0.00%	0.00%
Phenol, styrenated	262-975-0	61788-44-1	61788441	-	-	4494	3.99	0.55	3	3.27	0.58		-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
[1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[tert-butyl] pe	246-678-3	25155-25-3	25155253	-	-	4495	5.88		1				-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
Fatty acids, C12-20 and C12-20-unsatd., 2-ethylhexyl esters	292-811-3	91001-42-2	91001422	-	-	4496							-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
Fatty acids, coco, triesters with trimethylolpropane	287-640-6	85566-29-6	85566296	-	-	4497	5.83	1.06	3	4.83	1.06		-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
neodecanoyl chloride	254-875-0	40292-82-8	40292828	-	-	4498	3.93	1.05	3	2.93	1.05		-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
Urea, reaction products with formaldehyde, glyoxal and methan	296-665-1	92908-36-6	92908366	-	-	4499	5.68	0.58	3	4.68	0.58		-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
606-203-6	606-203-6	1902-01-8	1902018	-	-	4500	6.50		1				-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
600-444-0	600-444-0	103513-05-9	103513059	-	-	4501							-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
Fatty acids, C12-14	292-771-7	90990-10-6	90990106	-	-	4502	3.73	0.21	3	2.73	0.21		-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
629-757-0	629-757-0	1224966-15-7	1224966157	-	-	4503	2.93	0.59	3	1.93	0.59		-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
Benzenesulfonic acid, mono-C11-13-branched alkyl derivs.	271-807-5	68608-88-8	68608888	-	-	4504	4.05		2				-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
Fusel oil	232-395-2	8013-75-0	8013750	-	-	4505	6.46	0.82	4	5.62	1.21		-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
605-717-8	605-717-8	174333-80-3	174333803	-	-	4506	3.64	0.70	3	2.64	0.70		-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
4,4'-Isopropylidenediphenol, ethoxylated	500-082-2	32492-61-8	32492618	-	-	4507	4.92	0.55	3	3.92	0.55		-4.1	-4.3	-5.7	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Alcohols, C7-9	266-417-7	66587-56-2	66587562	-	-	4508	3.84	0.55	3	2.84	0.55		-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
benzyl 3-isobutyryloxy-1-isopropyl-2,2-dimethylpropyl phthalate	240-920-1	16883-83-3	16883833	-	-	4509	3.88		1				-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
Alcohols, C12-13, ethoxylated	500-165-3	66455-14-9	66455149	-	-	4510	2.76	0.36	5	2.96	0.44		-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
Fatty acids, C18-unsatd., dimers, hydrogenated	500-231-1	68783-41-5	68783415	-	-	4511				2.93			-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
Hydrocarbons, C4, 1,3-butadiene-free, polymd., tetraisobutylene	297-628-2	93685-80-4	93685804	-	-	4512	7.67		1				-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
Fatty acids, C16-18 and C18-unsatd., mixed esters with adipic ac	292-832-8	91001-61-5	91001615	-	-	4513				5.04			-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
Eucalyptus globulus, ext.	283-406-2	84625-32-1	84625321	-	-	4514	4.78	0.80	3	3.78	0.80		-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
Amines, C12-18-alkyldimethyl	269-923-6	68391-04-8	68391048	-	-	4515	2.12	0.66	3	1.18	0.77		-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
4,4'-Isopropylidenediphenol, oligomeric reaction products with 1	500-089-0	36425-15-7	36425157	-	-	4516							-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
Fatty acids, C18-unsatd., trimers	500-239-5	68937-90-6	68937906	-	-	4517				2.93			-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
Boric acid (H3BO3), reaction products with ethanolamine	302-207-4	94095-04-2	94095042	-	-	4518	5.08	0.51	3	4.08	0.51		-4.1	-4.3	-5.7	0.00%	0.00%	0.00%
Poly[oxy(methyl-1,2-ethanediyl)],α-butyl-ω-hydroxy-	500-003-1	9003-13-8	9003138	-	-	4519	4.97	0.52	5	4.56	0.32		-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
Rosin, maleated	232-480-4	8050-28-0	8050280	-	-	4520	4.19	0.28	3	4.18	0.78		-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
Fatty acids, sunflower-oil, conjugated	273-195-5	68953-27-5	68953275	-	-	4521							-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
diisodecyl azelate	249-044-4	28472-97-1	28472971	-	-	4522							-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
diisodecyl adipate	248-299-9	27178-16-1	27178161	-	-	4523							-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
4,4'-Isopropylidenediphenol, oligomeric reaction products with 1	500-101-4	38294-64-3	38294643	-	-	4524	4.41	0.45	3	3.41	0.45		-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
Nonylphenol, branched, ethoxylated	500-209-1	68412-54-4	68412544	-	-	4525	2.15	0.44	4	1.15	0.44		-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
Soaps, stocks, vegetable-oil, acidulated	273-179-8	68952-95-4	68952954	-	-	4526	4.64	0.75	4	3.64	0.75		-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
Ionone, methyl-	215-635-0	1335-46-2	1335462	-	-	4527	4.15	0.78	3	3.15	0.78		-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, chl	273-501-7	68987-63-3	68987633	-	-	4528	5.40		2	3.00			-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
627-083-1	627-083-1	244235-47-0	244235470	-	-	4529	4.17	1.62	3	3.17	1.62		-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
Resin acids and Rosin acids, calcium zinc salts	269-825-3	68334-35-0	68334350	-	-	4530	4.13	1.14	3	3.79	1.27		-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
Fatty acids, C14-18 and C16-18-unsatd., barium salts	305-998-4	95465-85-3	95465853	-	-	4531	5.42	0.57	3	3.80	0.22		-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
Alkenes, C11-12, hydroformylation products, distn. residues	292-427-6	90622-27-8	90622278	-	-	4532	5.30	0.31	3	4.30	0.31		-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholi	272-712-1	68909-77-3	68909773	-	-	4533	5.46	0.73	3	4.46	0.73		-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
Phenol, isobutylenated, phosphate (3:1)	273-065-8	68937-40-6	68937406	-	-	4534	3.44	0.50	3	2.00	0.47		-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
tris(methylphenyl) phosphate	215-548-8	1330-78-5	1330785	-	-	4535	3.30	1.18	22	1.43	0.99	7	-4.1	-4.4	-5.7	0.00%	0.00%	0.00%
Fatty acids, C18-unsatd., dimers, oligomeric reaction products w	500-191-5	68082-29-1	68082291	-	-	4536	3.80	0.14	3	3.06	0.47		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
tricyclodecanedimethanol	248-096-5	26896-48-0	26896480	-	-	4537	5.38	0.22	3	4.38	0.22		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
Quaternary ammonium compounds, di-C12-18-alkyldimethyl, ch	269-924-1	68391-05-9	68391059	-	-	4538	2.48	0.32	3	1.62	0.24		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
Fatty acids, C16-22	268-103-5	68002-88-0	68002880	-	-	4539							-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
Oils, animal, sulfated, sodium salts	304-835-4	94279-90-0	94279900	-	-	4540	5.43	0.55	3	4.43	0.55		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
Oils, vegetable, sulfated	263-113-6	61790-19-0	61790190	-	-	4541	5.43	0.55	3	4.43	0.55		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
Octadecanoic acid, branched and linear	269-214-1	68201-37-6	68201376	-	-	4542	6.03	1.10	3	5.03	1.10		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
Decanoic acid, mixed esters with dipentaerythritol, octanoic acic	270-470-1	68441-66-7	68441667	-	-	4543							-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
614-114-9	614-114-9	67746-08-1	67746081	-	-	4544	5.10	1.38	3	4.10	1.38		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
Glycerides, C16-22	268-083-8	68002-70-0	68002700	-	-	4545	5.83	0.55	3	4.83	0.55		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
629-725-6	629-725-6	1226892-45-0	1226892450	-	-	4546	2.90	0.58	3	1.90	0.58		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
Reaction mass of ethyl (2S,3S)-3,4-dibromo-2-methylbutanoate a	700-225-0	1160806-44-9	1160806449	-	-	4547	4.50		1				-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
605-322-0	605-322-0	163292-61-3	163292613	-	-	4548							-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
1-hydroxy-2-methylpentan-3-one	939-893-5	27970-79-2	27970792	-	-	4549							-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
1,4-anhydro-2,5-dideoxy-2-(methoxycarbonyl)-1-thiopent-3-ulos	619-801-7	66319-07-1	66319071	-	-	4550							-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
Benzene, butyl-, branched and linear	270-126-0	68411-44-9	68411449	-	-	4551	3.32	0.18	3	2.32	0.18		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
Benzenesulfonic acid, mono-C11-13-branched alkyl derivs., calci	273-234-6	68953-96-8	68953968	-	-	4552	4.40	0.54	3	2.62	0.39		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
Fatty acids, C16-18, C12-18-alkyl esters	306-083-2	95912-87-1	95912871	-	-	4553	5.83	1.22	3	4.83	1.22		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
Fatty acids, C16-18, isotridecyl esters	306-084-8	95912-88-2	95912882	-	-	4554	5.00		1				-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
629-705-7	629-705-7	1228186-15-9	1228186159	-	-	4555	3.13	0.31	3	2.13	0.31		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
Cinnamomum zeylanicum, ext.	283-479-0	84649-98-9	84649989	-	-	4556	3.22		2				-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
629-850-6	629-850-6	1245638-61-2	1245638612	-	-	4557	3.90	0.41	3	2.78	0.76		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
sorbitan laurate	215-663-3	1338-39-2	1338392	-	-	4558	4.94	0.70	3	3.94	0.70		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
Tar acids, xylenol fraction	284-895-5	84989-06-0	84989060	-	-	4559	4.29	0.35	3	3.46	0.43		-4.2	-4.4	-5.8	0.00%	0.00%	0.00%
triisotridecyl phosphite	278-758-9	77745-66-5	77745665	-	-	4560							-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
Ethanol, 2,2'-iminobis-, N-(C13-15-branched and linear alkyl) der	308-208-6	97925-95-6	97925956	-	-	4561	2.21	0.91	3	1.21	0.91		-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
diisotridecyl phthalate	248-368-3	27253-26-5	27253265	-	-	4562	3.17	0.52	3	2.53	0.55		-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
methyl-1H-benzotriazole	249-596-6	29385-43-1	29385431	-	-	4563	4.87	0.44	3	3.59	0.57		-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
diisodecyl phenyl phosphite	247-098-3	25550-98-5	25550985	-	-	4564	3.60		2				-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
dihydro-3-(tetrapropenyl)furan-2,5-dione	247-781-6	26544-38-7	26544387	-	-	4565	4.59		2				-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
2,4,7,9-tetramethyldec-5-yne-4,7-diol	204-809-1	126-86-3	126863	-	-	4566	4.57	0.32	3	3.50	0.73		-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
Castor oil, sulfated, sodium salt	269-123-7	68187-76-8	68187768	-	-	4567	5.01	0.44	3	3.98	0.55		-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
2,2'-(C16-18 (evennumbered, C18 unsaturated) alkyl imino) dietl	620-540-6	1218787-32-6	1218787326	-	-	4568	1.97	0.71	3	0.97	0.71		-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
Phosphorodithioic acid, mixed O,O-bis(iso-Bu and pentyl) esters,	270-608-0	68457-79-4	68457794	-	-	4569	4.29	0.37	3	3.29	0.37		-4.2	-4.5	-5.8	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
4-tert-butylcyclohexyl acetate	250-954-9	32210-23-4	32210234	-	-	4570	4.06	0.25	3	3.06	0.25		-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
Acetic acid, chloro-, sodium salt, reaction products with 4,5-dihy	271-794-6	68608-66-2	68608662	-	-	4571	4.33	0.82	3	3.33	0.82		-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
hexahydromethylphthalic anhydride	247-094-1	25550-51-0	25550510	-	-	4572	5.34	0.29	3	4.34	0.29		-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
614-668-1	614-668-1	68610-97-9	68610979	-	-	4573							-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
Decanoic acid, mixed diesters with octanoic acid and propylene	271-516-3	68583-51-7	68583517	-	-	4574	4.11	1.82	3	3.11	1.82		-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
1-Butene, chlorinated, epoxidized, distn. residues	304-781-1	94279-37-5	94279375	-	-	4575							-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
sorbitan stearate	215-664-9	1338-41-6	1338416	-	-	4576				4.20			-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
Amylase, gluco-	232-877-2	9032-08-0	9032080	-	-	4577	5.62	0.28	3	4.62	0.28		-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
641-136-6	641-136-6	1160164-88-4	1160164884	-	-	4578	5.50		3	4.50			-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
Amines, di-C12-18-alkylmethyl	270-418-8	68439-75-8	68439758	-	-	4579	2.60	1.00	3	1.60	1.00		-4.2	-4.5	-5.8	0.00%	0.00%	0.00%
Phenol, dodecyl-, sulfurized, calcium salts	272-486-4	68855-45-8	68855458	-	-	4580	6.21	0.41	3	5.21	0.41		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
extract residues (coal tar), high-temperature, naphthalene oil alk	310-256-8	140362-65-8	140362658	-	-	4581	4.36		1				-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
Amylase, α-	232-565-6	9000-90-2	9000902	-	-	4582	5.27	1.05	3	4.27	1.05		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
Ethanol, 2,2'-iminobis-, N-C12-18-alkyl derivs.	276-014-8	71786-60-2	71786602	-	-	4583	2.50	0.43	3	1.43	0.61		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
Fatty acids, tall-oil, Bu esters	267-028-5	67762-63-4	67762634	-	-	4584	5.11		2	5.00			-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
605-318-9	605-318-9	163206-31-3	163206313	-	-	4585	5.75		1				-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
Resin acids and Rosin acids, maleated, sodium salts	269-228-8	68201-60-5	68201605	-	-	4586	4.19	0.28	3	4.18	0.78		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
Oils, animal, sulfonated, sodium salts	305-979-0	95371-11-2	95371112	-	-	4587	5.35	0.53	3	4.35	0.53		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
4,4'-Methylenediphenyl diisocyanate, oligomeric reaction produ	500-439-2	159168-82-8	159168828	-	-	4588	6.37	0.26	3	5.37	0.26		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
2-Propenenitrile, reaction products with ethylenediamine, hydro	272-727-3	68909-99-9	68909999	-	-	4589	5.06	0.36	3	3.87	0.60		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
tridecylamine, branched and linear	289-185-9	86089-17-0	86089170	-	-	4590	1.87	0.74	3	1.04	1.01		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
3-[C13-(branched)-alkyloxy]propionitrile	700-399-8	947522-81-8	947522818	-	-	4591							-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
Nitriles, C16-18	268-079-6	68002-65-3	68002653	-	-	4592							-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
Linseed oil, epoxidized	232-401-3	8016-11-3	8016113	-	-	4593							-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
Rosin, oligomers	500-163-2	65997-05-9	65997059	-	-	4594	4.09	1.16	3	3.77	1.29		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
Alkanes, C10-13, chloro	287-476-5	85535-84-8	85535848	-	-	4595	3.88	1.63	12	1.69	0.72	11	-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl 3,4,5,6-tetrabromoph	243-885-0	20566-35-2	20566352	-	-	4596	3.96	0.16	3	2.96	0.16		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
630-399-2	630-399-2	130169-56-1	130169561	-	-	4597	2.25	0.78	3	1.48	0.71		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
614-264-5	614-264-5	68081-77-6	68081776	-	-	4598							-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
Fatty acids, C14-22	270-298-7	68424-37-3	68424373	-	-	4599	4.78	1.68	3	3.78	1.68		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
Glycerides, C8-18 and C18-unsatd. mono- and di-, acetates	293-170-2	91052-13-0	91052130	-	-	4600	4.88	0.68	3	3.88	0.68		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
Octadecan-1-ol, ethoxylated	500-017-8	9005-00-9	9005009	-	-	4601	3.20	0.51	3	1.83	0.47		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
Fatty acids, C8-18 and C18-unsatd., esters with neopentyl glycol	286-072-6	85186-86-3	85186863	-	-	4602	6.00		1	2.32			-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
Fatty acids, palm-oil, hydrogenated	282-486-6	84238-17-5	84238175	-	-	4603	5.00		1				-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
Amines, N-C12-18-alkyltrimethylenedi-	268-957-9	68155-37-3	68155373	-	-	4604	2.88	2.09	3	1.88	2.09		-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
Tar, wood	294-436-0	91722-33-7	91722337	-	-	4605							-4.3	-4.5	-5.9	0.00%	0.00%	0.00%
N-(2-hydroxyethyl)stearamide	203-883-2	111-57-9	111579	-	-	4606	3.94	0.61	3	2.85	0.65		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
603-894-6	603-894-6	135108-88-2	135108882	-	-	4607	4.56	0.29	3	3.36	0.62		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
Benzenesulfonic acid, propenated, calcium salt, overbased	271-877-7	68610-84-4	68610844	-	-	4608	6.19	0.60	3	5.19	0.60		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
trixylyl phosphate	246-677-8	25155-23-1	25155231	-	-	4609	3.62	1.32	4	1.65	0.74		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
Ethanol, 2-amino-, reaction products with ammonia, 1-piperazin	296-543-8	92731-41-4	92731414	-	-	4610	5.16	0.84	3	4.34	0.89		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
Alkenes, C13-14, hydroformylation products, distn. residues	292-429-7	90622-29-0	90622290	-	-	4611	5.30	0.35	3	4.30	0.35		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
Hexanoic acid, 2-ethyl-, C16-18-alkyl esters	291-445-1	90411-68-0	90411680	-	-	4612							-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
Gases (petroleum), extractive, C3-5, butene-isobutylene-rich	270-732-5	68477-42-9	68477429	-	-	4613	4.19	0.23	3	3.19	0.23		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
Pentaerythritol, ethoxylated, esters with acrylic acid	500-111-9	51728-26-8	51728268	-	-	4614	4.47	0.85	3	3.47	0.85		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate, oligon	500-287-7	103170-26-9	103170269	-	-	4615	5.70		1				-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
dodecyl oleate	252-862-4	36078-10-1	36078101	-	-	4616	5.67	0.25	3	4.67	0.25		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
Toluene diisocyanate, oligomeric reaction products with water	500-299-2	110839-12-8	110839128	-	-	4617							-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
603-931-6	603-931-6	135800-37-2	135800372	-	-	4618	5.36		1				-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
Acid chlorides, coco	269-133-1	68187-89-3	68187893	-	-	4619	4.05	1.02	3	4.18	0.90		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
ethanol, 2-methoxy-, manufacture of, by-products from, esters v	310-290-3	161907-80-8	161907808	-	-	4620	5.96	0.46	3	4.96	0.46		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
Acetic acid, oxo-, sodium salt, reaction products with ethylenedi	283-042-4	84539-54-8	84539548	-	-	4621	5.39	0.70	4	4.39	0.70		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
Fatty acids, C16-18 and C18-unsatd., tetraesters with pentaeryth	271-694-2	68604-44-4	68604444	-	-	4622	5.72	0.76	3	4.72	0.76		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
Urea, reaction products with formaldehyde and glyoxal	296-664-6	92908-35-5	92908355	-	-	4623	5.74	0.70	3	4.74	0.70		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
zinc O,O,O',O'-tetrakis(1,3-dimethylbutyl) bis(phosphorodithioat	218-679-9	2215-35-2	2215352	-	-	4624	4.29	0.37	3	3.29	0.37		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
Propylidynetrimethanol, propoxylated, reaction products with a	500-105-6	39423-51-3	39423513	-	-	4625							-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
694-876-7	694-876-7	1345668-41-8	1345668418	-	-	4626	3.99	0.49	3	3.32	0.23		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
620-539-0	620-539-0	1218787-30-4	1218787304	-	-	4627	2.04	0.59	3	1.04	0.59		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
Glycerides, palm-oil mono-, hydrogenated, acetates	297-462-0	93572-32-8	93572328	-	-	4628	4.16		2				-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
601-101-8	601-101-8	111497-86-0	111497860	-	-	4629	5.28	0.37	3	4.28	0.37		-4.3	-4.6	-5.9	0.00%	0.00%	0.00%
Tetrakis(hydroxymethyl)phosphonium chloride, oligomeric react	500-057-6	27104-30-9	27104309	-	-	4630	3.94	1.77	3	3.40	1.13		-4.3	-4.6	-6.0	0.00%	0.00%	0.00%
Fatty acids, C5-10, esters with dipentaerythritol	275-093-6	70983-72-1	70983721	-	-	4631	5.75	0.63	3	4.75	0.63		-4.3	-4.6	-6.0	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Cocoa, ext.	283-480-6	84649-99-0	84649990	-	-	4632	4.47		1				-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-indenyl propionate	272-805-7	68912-13-0	68912130	-	-	4633	3.85	0.19	3	2.85	0.19		-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
hexyl D-glucoside	259-217-6	54549-24-5	54549245	-	-	4634	5.75	0.21	3	4.81	0.25		-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
696-026-0	696-026-0	1395383-69-3	1395383693	-	-	4635	4.50	0.29	3	3.52	0.68		-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
Fatty acids, coco, 2-sulfoethyl esters, sodium salts	263-052-5	61789-32-0	61789320	-	-	4636	4.20	0.50	3	3.11	0.86		-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
Fatty acids, C8-18 and C18-unsatd., esters with trimethylolpropa	286-075-2	85186-89-6	85186896	-	-	4637	6.34	1.13	3	5.34	1.13		-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
zinc bis(O,O-diisooctyl) bis(dithiophosphate)	249-109-7	28629-66-5	28629665	-	-	4638	5.11	0.89	3	4.11	0.89		-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
diisooctyl adipate	215-553-5	1330-86-5	1330865	-	-	4639	5.73	0.77	3	4.73	0.77		-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
Glycerol, ethoxylated	500-075-4	31694-55-0	31694550	-	-	4640				4.00			-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
Benzenamine, reaction products with aniline hydrochloride and	309-912-6	101357-15-7	101357157	-	-	4641				1.32			-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
benzenesulfonic acid, 2,2'-(1,2-ethenediyl)bis[5-nitro-, disodium	215-397-8	1325-54-8	1325548	-	-	4642	5.80		1				-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
800-353-8	800-353-8	1379524-06-7	1379524067	-	-	4643	1.94	1.02	3	0.94	1.02		-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
603-046-5	603-046-5	125301-84-0	125301840	-	-	4644				4.00			-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
Decanoic acid, mixed esters with heptanoic acid, octanoic acid a	268-596-7	68130-53-0	68130530	-	-	4645	6.17	1.00	3	5.17	1.00		-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
Glycerol, ethoxylated, esters with acrylic acid	500-322-6	144086-03-3	144086033	-	-	4646	4.61	0.68	3	3.61	0.68		-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
Propanenitrile, 3-amino-, N-tallow alkyl derivs.	272-268-9	68784-70-3	68784703	-	-	4647							-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
sorbitan palmitate	247-568-8	26266-57-9	26266579	-	-	4648				4.20			-4.4	-4.6	-6.0	0.00%	0.00%	0.00%
ε-Caprolactone, oligomeric reaction products with propylidynetr	500-099-5	37625-56-2	37625562	-	-	4649	5.56	0.56	3	4.59	0.34		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
bis(4-tert-butylcyclohexyl) peroxydicarbonate	239-557-1	15520-11-3	15520113	-	-	4650	5.02	0.72	3	4.02	0.72		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
614-283-9	614-283-9	68127-59-3	68127593	-	-	4651	5.14		1				-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
4,4'-Isopropylidenedicyclohexanol, oligomeric reaction products	500-070-7	30583-72-3	30583723	-	-	4652	4.06		1				-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
Resin acids and Rosin acids, hydrogenated, esters with pentaery	264-848-5	64365-17-9	64365179	-	-	4653	6.20	0.63	3	5.20	0.63		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
N-butyl-2,2,6,6-tetramethylpiperidin-4-amine, oligomeric reactic	500-311-6	120498-03-5	120498035	-	-	4654	3.65		2				-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
Phenol, reaction products with 1-bromo-4-phenoxybenzene and	700-709-1	1264747-45-6	1264747456	-	-	4655	5.64	0.26	3	4.64	0.26		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
Benzenesulfonic acid, 4-C10-13-sec-alkyl derivs., compds. with 2	284-664-9	84961-74-0	84961740	-	-	4656	4.03	0.67	4	3.13	0.51		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
Sulfuric acid, mono-C16-18-alkyl esters, sodium salts	273-258-7	68955-20-4	68955204	-	-	4657	4.61	0.48	3	3.78	0.89		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
629-732-4	629-732-4	1224966-13-5	1224966135	-	-	4658	2.90	0.58	3	1.90	0.58		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
800-984-9	800-984-9	1428547-35-6	1428547356	-	-	4659	2.25	0.78	3	1.48	0.71		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
1-Pentene, chlorinated, epoxidized, distn. residues	304-798-4	94279-53-5	94279535	-	-	4660							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
Isotridecanol, ethoxylated	500-241-6	69011-36-5	69011365	-	-	4661	3.38	0.20	3	2.38	0.20		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
609-993-0	609-993-0	42131-25-9	42131259	-	-	4662				5.00			-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
anhydro-D-glucitol trioleate	247-569-3	26266-58-0	26266580	-	-	4663	6.79	0.59	3	5.79	0.59		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
700-481-3	700-481-3	10257-32-6	10257326	-	-	4664							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
Rosin amine distillation fraction of disproportionated, ammoniat	801-966-3	12698-87-2	12698872	-	-	4665	2.40		1				-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
2-piperidin-2-ylethanol	216-059-2	1484-84-0	1484840	-	-	4666							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
D-Glucopyranose, oligomers, C12-14-alkyl glycosides	500-395-4	157707-88-5	157707885	-	-	4667							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
ethyl 2-(ethoxymethylene)-4,4-difluoro-3-oxobutanoate	619-794-0	176969-33-8	176969338	-	-	4668							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
1,2,3,4-tetrahydro-1-naphthylamine	218-712-7	2217-40-5	2217405	-	-	4669	4.25		1				-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
1-ethylpyrrolidin-2-ylmethylamine	247-466-3	26116-12-1	26116121	-	-	4670							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
609-333-1	609-333-1	37143-54-7	37143547	-	-	4671	4.80	0.25	3	3.94	0.26		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
methylpentane	639-864-4	43133-95-5	43133955	-	-	4672	4.33	0.20	3	3.33	0.20		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
805-389-8	805-389-8	500011-91-6	500011916	-	-	4673							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
Methyl 3-chloro-2-fluoropropanoate	627-096-2	55900-27-1	55900271	-	-	4674							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
2,2'-(ethane-1,2-diyldiimino)bis[(2-hydroxy-5- sulfophenyl)acetic	611-514-5	57368-07-7	57368077	-	-	4675							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
2-methylcyclohexanol, mixed isomers	209-512-0	583-59-5	583595	-	-	4676							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
Fatty acids, tall-oil, ethoxylated	500-150-1	61791-00-2	61791002	-	-	4677							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
1-(3-methoxyphenyl)ethanamine	700-849-3	62409-13-6	62409136	-	-	4678	4.72		1				-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
1-(4-Methoxyphenyl)ethanamine	700-847-2	6298-96-0	6298960	-	-	4679	4.72		1				-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
613-701-7	613-701-7	6485-45-6	6485456	-	-	4680	5.33	0.18	3	4.41	0.16		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
Tar bases, coal, crude	266-018-8	65996-84-1	65996841	-	-	4681	3.76		2				-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
Sulfonic acids, alkane, sodium salts	271-774-7	68608-15-1	68608151	-	-	4682	4.00		1				-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
N-{1-cyano-2-[5-cyano-2-(trifluoromethyl)phenoxy]-1-methyleth	632-606-1	851976-50-6	851976506	-	-	4683							-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
Fatty acids, tall-oil, compds. with N-[3-(dimethylamino)propyl]ta	295-714-4	92128-22-8	92128228	-	-	4684	2.68	0.57	3	1.99	0.40		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
2-Propenoic acid, butyl ester, reaction products with butadiene,	300-339-7	93925-37-2	93925372	-	-	4685	4.48	0.43	3	3.26	0.56		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Pr) e	272-723-1	68909-93-3	68909933	-	-	4686	3.73	0.50	3	2.78	0.61		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
Tridecanamine, N-tridecyl-, branched and linear	309-798-8	101012-97-9	101012979	-	-	4687	3.32	0.95	3	3.30	0.40		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
1,3,4-Thiadiazolidine-2,5-dithione, reaction products with hydro	293-927-7	91648-65-6	91648656	-	-	4688	5.28	0.56	3	4.59	0.61		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
Naphthenic acids, reaction products with diethylenetriamine	268-610-1	68131-13-5	68131135	-	-	4689	3.21	0.54	3	2.21	0.54		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
diisopropylbenzene	246-835-6	25321-09-9	25321099	-	-	4690	2.92	0.37	3	1.98	0.21		-4.4	-4.7	-6.0	0.00%	0.00%	0.00%
604-608-2	604-608-2	147853-32-5	147853325	-	-	4691	5.48	1.14	3	4.48	1.14		-4.4	-4.7	-6.1	0.00%	0.00%	0.00%
3,7-dimethylnona-1,6-dien-3-ol	233-732-6	10339-55-6	10339556	-	-	4692	4.41	0.17	3	3.22	0.23		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
696-616-8	696-616-8	1268344-02-0	1268344020	-	-	4693	2.36	0.17	3	1.36	0.17		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
606-330-7	606-330-7	195008-76-5	195008765	-	-	4694	4.24	0.68	3	3.24	0.68		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
sucrose di(acetate) hexaisobutyrate	204-771-6	126-13-6	126136	-	-	4695	3.92	1.27	3	2.92	1.27		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Alcohols, C9-11, branched and linear, ethoxylated, sulfates, amm	500-464-9	160901-27-9	160901279	-	-	4696	4.65	0.43	3	3.65	0.43		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
629-765-4	629-765-4	1226892-44-9	1226892449	-	-	4697	2.94	0.54	3	2.31	0.23		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Fatty acids, C8-10, C12-18-alkyl esters	306-082-7	95912-86-0	95912860	-	-	4698	5.67	0.75	3	4.67	0.75		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Cellulase	232-734-4	9012-54-8	9012548	-	-	4699	5.24	0.24	3	4.24	0.24		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
2-propylheptyl acrylate	604-669-5	149021-58-9	149021589	-	-	4700	4.17	0.77	3	3.17	0.77		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
1,2,3,6-Tetrahydrophthalic anhydride, oligomeric reaction produ	500-091-1	36621-20-2	36621202	-	-	4701	4.52		1				-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
2,4,6-tri-sec-butylphenol	227-572-6	5892-47-7	5892477	-	-	4702	3.55		2				-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Soaps, stocks, acidulated	271-768-4	68607-87-4	68607874	-	-	4703							-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Quaternary ammonium compounds, bis(hydrogenated tallow all	272-745-1	68910-55-4	68910554	-	-	4704	5.10		1				-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Rosin, fumarated, reaction products with formaldehyde	305-795-0	95009-65-7	95009657	-	-	4705	6.17	0.58	3	5.17	0.58		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Humic acids, sodium salts	268-608-0	68131-04-4	68131044	-	-	4706	5.48	0.15	3	4.48	0.15		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Phosphoric acid, 2-ethylhexyl ester	235-741-0	12645-31-7	12645317	-	-	4707	5.15	0.57	3	4.31	0.36		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Pentaerythritol, ethoxylated	500-071-2	30599-15-6	30599156	-	-	4708	5.42	0.25	3	4.42	0.25		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Benzenamine, N-phenyl-, reaction products with styrene and 2,4	272-940-1	68921-45-9	68921459	-	-	4709	5.20		2				-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Mentha arvensis, ext.	290-058-5	90063-97-1	90063971	-	-	4710	3.43	0.05	3	2.43			-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
1-Octadecanol, phosphate, potassium salt	273-489-3	68987-29-1	68987291	-	-	4711	5.50		3	4.50			-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Fatty acids, C8-10, tetraesters with pentaerythritol	287-827-2	85586-24-9	85586249	-	-	4712	6.19	0.79	3	5.19	0.79		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Lemon, ext.	284-515-8	84929-31-7	84929317	-	-	4713	3.20	0.75	3	2.20	0.75		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Fatty acids, C16-18, Bu esters	287-039-9	85408-76-0	85408760	-	-	4714	6.16	1.09	3	5.16	1.09		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
2,4-Pentanedione, peroxide	253-384-9	37187-22-7	37187227	-	-	4715	3.79		2				-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Oils, fish, sulfated, sodium salts	262-992-3	61788-64-5	61788645	-	-	4716	5.43	0.55	3	4.43	0.55		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Fatty acids, C16-18 and C18 unsatd., triesters with trimethylolpr	268-092-7	68002-78-8	68002788	-	-	4717				5.04			-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
Soybean oil, deodorizer distillate	272-211-8	68783-88-0	68783880	-	-	4718	5.00		1				-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
α,α,α',α'-tetramethylxylene-α,α-diol	248-256-4	27138-01-8	27138018	-	-	4719	5.59	0.10	3	4.59	0.10		-4.5	-4.7	-6.1	0.00%	0.00%	0.00%
614-637-2	614-637-2	68603-75-8	68603758	-	-	4720	2.02	0.45	3	1.02	0.45		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
Fatty acids, C6-18, triesters with trimethylolpropane	293-035-8	91050-88-3	91050883	-	-	4721				6.07			-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
Castor oil, dehydrated	264-705-7	64147-40-6	64147406	-	-	4722	5.83	0.58	3	4.83	0.58		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
800-526-8	800-526-8	1273322-45-4	1273322454	-	-	4723	2.53	0.49	3	1.66	0.61		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
disodium oxybis[methylbenzenesulphonate]	277-242-0	73037-34-0	73037340	-	-	4724	5.05		1				-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
Amines, C11-14-branched alkyl, monohexyl and dihexyl phospha	279-632-6	80939-62-4	80939624	-	-	4725	3.47	0.49	3	2.76	0.50		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
605-143-8	605-143-8	158318-67-3	158318673	-	-	4726	5.75	0.74	3	4.75	0.74		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
601-566-7	601-566-7	118800-30-9	118800309	-	-	4727	4.13	0.56	3	3.13	0.56		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
Aromatic hydrocarbons, C6-10, C8-rich	292-697-5	90989-41-6	90989416	-	-	4728	3.30	0.22	3	2.30	0.22		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
Fatty acids, C8-18 and C18-unsatd., esters with pentaerythritol	285-202-9	85049-33-8	85049338	-	-	4729							-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
Alcohols, C9-11, branched and linear, ethoxylated	500-446-0	160901-09-7	160901097	-	-	4730							-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
4,4'-Isopropylidenediphenol, oligomeric reaction products with 1	500-180-5	67989-52-0	67989520	-	-	4731							-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
800-838-4	800-838-4	1384855-91-7	1384855917	-	-	4732	4.25	0.22	3	3.40	0.11		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
Soybean oil, epoxidized, acrylate	294-415-6	91722-14-4	91722144	-	-	4733	4.42		1				-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
Ethylenediamine, ethoxylated and propoxylated	500-047-1	26316-40-5	26316405	-	-	4734	5.74	1.16	3	4.23	0.67		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
decene	246-870-7	25339-53-1	25339531	-	-	4735	3.32	1.28	3	3.84	2.11		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
608-670-1	608-670-1	31831-53-5	31831535	-	-	4736	5.18	0.30	3	4.23	0.28		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
Alcohols, C8-14, γ-ω-perfluoro	269-927-8	68391-08-2	68391082	-	-	4737	2.90	0.28	3	1.90	0.28		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
triisodecyl phosphite	246-998-3	25448-25-3	25448253	-	-	4738							-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
Fatty acids, dehydrated castor-oil	263-061-4	61789-45-5	61789455	-	-	4739	5.78	1.19	3	4.78	1.19		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
9-Octadecenoic acid (Z)-, monoester with 1,2,3-propanetriol este	264-092-6	63310-16-7	63310167	-	-	4740	5.40	1.91	3	4.40	1.91		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
609-946-4	609-946-4	41637-38-1	41637381	-	-	4741	4.39		2				-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
Petrolatum (petroleum), oxidized, calcium salt	270-348-8	68425-34-3	68425343	-	-	4742	6.17	1.10	3	5.17	1.10		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
Hydrocarbons, terpene processing by-products	273-309-3	68956-56-9	68956569	-	-	4743	3.56	0.16	3	2.56	0.16		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
614-279-7	614-279-7	68122-64-5	68122645	-	-	4744	5.45	1.28	3	4.45	1.28		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
619-057-3	619-057-3	94667-33-1	94667331	-	-	4745	2.32	0.40	3	1.39	0.47		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
Fatty acids, C5-9, tetraesters with pentaerythritol	267-022-2	67762-53-2	67762532	-	-	4746	4.66	1.14	3	3.66	1.14		-4.5	-4.8	-6.1	0.00%	0.00%	0.00%
1,2-Benzenedicarboxylic acid, di-C8-10-alkyl esters	275-809-7	71662-46-9	71662469	-	-	4747	3.01	0.77	3	2.64	0.67		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
616-261-4	616-261-4	75782-87-5	75782875	-	-	4748	3.92		2				-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
Extract residues (coal), tar oil alk.	266-021-4	65996-87-4	65996874	-	-	4749	4.36		1				-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
2,2,4,4-tetramethylcyclobutane-1,3-diol, mixed isomers	221-140-0	3010-96-6	3010966	-	-	4750	5.54		3	4.54			-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
Phenol, dodecyl-, branched, sulfurized	306-115-5	96152-43-1	96152431	-	-	4751	6.16	0.40	3	5.16	0.40		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
1,2,3-propanetriyl trioleate	204-534-7	122-32-7	122327	-	-	4752				4.00			-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
Resin acids and Rosin acids, reaction products with formaldehyd	295-855-1	92129-53-8	92129538	-	-	4753	4.13	1.14	3	3.79	1.27		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
Castor oil, ethoxylated	500-151-7	61791-12-6	61791126	-	-	4754							-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
Soybean oil, epoxidized, ether with ethylene glycol	287-836-1	85586-34-1	85586341	-	-	4755	6.92	1.15	3	4.61	1.52		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Reaction products of benzene-1,4-diamine and methyl 2,3,4,5-te	600-736-8	106276-80-6	106276806	-	-	4756	5.50		3	4.50			-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
Acacia mearnsi, ext., reaction products with ammonium chloride	285-077-0	85029-52-3	85029523	-	-	4757	4.36	0.33	3	3.36	0.33		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
Fatty acids, C14-18 and C16-18-unsatd., mixed esters with neope	286-078-9	85186-92-1	85186921	-	-	4758	6.17	0.76	3	5.17	0.76		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
Phosphoric acid, C16-18-alkyl esters, potassium salts	291-907-2	90506-45-9	90506459	-	-	4759	5.50		3	4.50			-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
2-[[2,2-bis[[(1-oxoallyl)oxy]methyl]butoxy]methyl]-2-ethyl-1,3-pr	302-434-9	94108-97-1	94108971	-	-	4760	3.10		2				-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
629-742-9	629-742-9	1226892-49-4	1226892494	-	-	4761	2.94	0.54	3	2.31	0.23		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
Fatty acids, C5-9, hexaesters with dipentaerythritol	267-021-7	67762-52-1	67762521	-	-	4762	5.83	0.58	3	4.83	0.58		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
Fatty acids, C14-18 and C16-18-unsatd., maleated	288-306-2	85711-46-2	85711462	-	-	4763	4.96	0.83	3	3.96	0.83		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
614-295-4	614-295-4	68131-40-8	68131408	-	-	4764	3.59	0.70	28	2.39	0.70		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
Polyphosphoric acids, esters with triethanolamine, sodium salts	268-625-3	68131-72-6	68131726	-	-	4765	6.15	0.79	3	5.15	0.79		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
Castor oil, oxidized	269-128-4	68187-84-8	68187848	-	-	4766	5.13	0.72	3	4.13	0.72		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
604-394-0	604-394-0	144086-02-2	144086022	-	-	4767	4.51	0.79	3	3.51	0.79		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
4,4'-Isopropylidenediphenol, oligomeric reaction products with 1	500-181-0	68002-42-6	68002426	-	-	4768							-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
titanium tetra(octanolate), branched and linear	281-199-3	83897-91-0	83897910	-	-	4769	4.31	0.26	3	3.31	0.26		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
607-759-2	607-759-2	25618-55-7	25618557	-	-	4770	7.73		1				-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
1,2-Benzenedicarboxylic acid, di-C6-10-alkyl esters	271-094-0	68515-51-5	68515515	-	-	4771	3.01	0.77	3	2.64	0.67		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
2-Propanol, 1,1'-[[3-[(3-aminopropyl)amino]propyl]imino]bis-, N-	307-276-4	97592-79-5	97592795	-	-	4772	1.95	0.53	3	1.20	0.44		-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
Phosphoric acid, dodecyl ester, potassium salt	254-414-3	39322-78-6	39322786	-	-	4773	6.19		2				-4.6	-4.8	-6.2	0.00%	0.00%	0.00%
Fatty acids, C16-18, 1,2-ethanediylbis(oxy-2,1-ethanediyl) esters	292-947-3	91031-45-7	91031457	-	-	4774	4.27	0.90	3	3.27	0.90		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
Amines, N-C12-14-alkyltrimethylenedi-	292-562-0	90640-43-0	90640430	-	-	4775	1.73	0.45	3	0.73	0.45		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
Protein hydrolyzates, vegetable	309-353-8	100209-45-8	100209458	-	-	4776							-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
2-Propenoic acid, γ-ω-perfluoro-C8-14-alkyl esters	288-003-5	85631-54-5	85631545	-	-	4777	2.96	0.35	3	1.96	0.35		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
Amines, di-C12-18-alkyl	268-899-4	68153-95-7	68153957	-	-	4778	2.71		2				-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
3,7,11-trimethyldodeca-1,6,10-trien-3-ol,mixed isomers	230-597-5	7212-44-4	7212444	-	-	4779	3.15	0.21	6	2.15	0.21		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
tetradecyl oleate	244-949-0	22393-85-7	22393857	-	-	4780	5.17	0.79	3	4.17	0.79		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
1,3-dihydro-4(or 5)-methyl-2H-benzimidazole-2-thione	258-904-8	53988-10-6	53988106	-	-	4781	4.36	0.66	3	3.36	0.66		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
615-086-0	615-086-0	70225-05-7	70225057	-	-	4782							-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
Acetic acid, oxo-, sodium salt, reaction products with cresol and	283-041-9	84539-53-7	84539537	-	-	4783	5.33	1.08	4	4.33	1.08		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
Fatty acids, C16-18 and C18-unsatd., compds. with triethanolam	270-279-3	68424-19-1	68424191	-	-	4784							-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
Docosanoic acid, ester with 1,2,3-propanetriol	278-717-5	77538-19-3	77538193	-	-	4785	6.07	0.97	3	5.07	0.97		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu) e	270-478-5	68442-22-8	68442228	-	-	4786	4.29	0.37	3	3.29	0.37		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
diisopropylbenzene hydroperoxide	247-988-1	26762-93-6	26762936	-	-	4787	3.81	0.35	3	2.81	0.35		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
Resin acids and Rosin acids, fumarated, esters with glycerol	307-051-0	97489-11-7	97489117	-	-	4788							-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
sodium N-(2-carboxyethyl)-N-(2-ethylhexyl)-β-alaninate	305-318-6	94441-92-6	94441926	-	-	4789	5.59	0.16	3	4.59	0.16		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
Amides, C16-18 and C18-unsatd., N,N-bis(hydroxyethyl)	271-653-9	68603-38-3	68603383	-	-	4790	3.65	0.48	3	2.65	0.38		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
4,4'-Methylenedianiline, oligomeric reaction products with 1-chl	500-062-3	28390-91-2	28390912	-	-	4791	3.89	0.79	3	2.89	0.79		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
Fatty acids, C16-18, tetraesters with pentaerythritol	293-029-5	91050-82-7	91050827	-	-	4792	5.72	0.76	3	4.72	0.76		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
694-886-1	694-886-1	1365095-43-7	1365095437	-	-	4793	5.64	0.99	3	4.64	0.99		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
614-523-2	614-523-2	68475-37-6	68475376	-	-	4794	6.20	0.63	3	5.20	0.63		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
tert-butyl peroxyneodecanoate	247-955-1	26748-41-4	26748414	-	-	4795	2.61	0.43	3	1.75	0.63		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
Tar acids, distn. residues	306-251-5	96690-55-0	96690550	-	-	4796							-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
Amines, C16-18-alkyldimethyl	269-915-2	68390-97-6	68390976	-	-	4797	2.12	0.66	3	1.18	0.77		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
Fatty acids, C12-16, esters with neopentyl glycol	286-081-5	85186-95-4	85186954	-	-	4798	6.17	0.76	3	5.17	0.76		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
Naphthalenesulfonic acids, branched and linear Bu derivs., sodiu	293-346-9	91078-64-7	91078647	-	-	4799	5.08	0.16	3	4.08	0.16		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
Alcohols, C6-24 and C6-24-unsatd., distn. residues	310-079-6	102242-48-8	102242488	-	-	4800	6.83	1.15	3	5.83	1.15		-4.6	-4.9	-6.2	0.00%	0.00%	0.00%
docosyl docosanoate	241-646-5	17671-27-1	17671271	-	-	4801							-4.6	-4.9	-6.3	0.00%	0.00%	0.00%
Glycerides, C16-18 mono-, di- and tri-, hydrogenated, citrates, pe	294-600-1	91744-38-6	91744386	-	-	4802							-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
606-078-8	606-078-8	186321-96-0	186321960	-	-	4803	2.81	0.55	3	2.03	0.74		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
800-660-7	800-660-7	1258274-08-6	1258274086	-	-	4804	5.15	0.49	3	4.15	0.49		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
Fatty acids, tall-oil, C12-15-alkyl esters, sulfated, sodium salts	270-307-4	68424-50-0	68424500	-	-	4805	5.03	0.55	3	4.10	0.56		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
Fatty acids, tallow, zinc salts	270-451-8	68440-34-6	68440346	-	-	4806	3.12	0.69	3	1.92	0.67		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
d-Glucose, ether with glycerol	309-496-6	100402-60-6	100402606	-	-	4807	6.32	0.13	3	5.32	0.13		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
610-877-7	610-877-7	52624-57-4	52624574	-	-	4808							-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
2,2-bis[[(1-oxoisooctadecyl)oxy]methyl]-1,3-propanediyl bis(isoo	263-423-1	62125-22-8	62125228	-	-	4809	5.63	0.19	3	4.63	0.19		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
Alcohols, C9-11, branched and linear, ethoxylated, sulfates, sodi	500-465-4	160901-28-0	160901280	-	-	4810	4.65	0.43	3	3.65	0.43		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
(1α,2β,4β,6α)-2,2,7-trimethyl-3-oxatricyclo[4.1.1.02,4]octane	250-938-1	32162-27-9	32162279	-	-	4811							-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
629-723-5	629-723-5	1190409-68-7	1190409687	-	-	4812							-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
806-510-7	806-510-7	1393571-43-1	1393571431	-	-	4813	5.50		3	4.50			-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
629-716-7	629-716-7	1211950-04-7	1211950047	-	-	4814	2.84	0.30	3	1.84	0.30		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
diisodecyl sebacate	249-047-0	28473-19-0	28473190	-	-	4815	6.50		3	5.50			-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
800-172-4	800-172-4	398141-87-2	398141872	-	-	4816	3.76	0.58	3	2.42	0.38		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
Butanedioic acid, sulfo-, 1-C12-18-alkyl esters, disodium salts	290-836-4	90268-36-3	90268363	-	-	4817	4.06	0.74	3	3.06	0.74		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Distillates (coal tar), pitch	309-855-7	101316-49-8	101316498	-	-	4818	4.70		2				-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
606-155-6	606-155-6	188831-96-1	188831961	-	-	4819	4.98	0.58	3	3.98	0.58		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
Phosphoric acid, octadecyl ester	254-466-7	39471-52-8	39471528	-	-	4820				0.48			-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
Amines, tallow alkyl, dodecylbenzenesulfonates	268-766-0	68139-94-6	68139946	-	-	4821							-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
Fatty acids, tall-oil, reaction products with formaldehyde and (Z)	272-789-1	68911-83-1	68911831	-	-	4822	3.49	0.45	3	2.49	0.45		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
Peptones, casein	293-428-4	91079-40-2	91079402	-	-	4823							-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
zinc bis[bis(tetrapropylenephenyl)] bis(hydrogen dithiophosphat	234-277-6	11059-65-7	11059657	-	-	4824	5.75	0.66	3	4.75	0.66		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
cyclohexane-1,4-dicarboxylic acid	214-068-6	1076-97-7	1076977	-	-	4825	5.22	0.43	3	4.22	0.43		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
4,4'-Isopropylidenediphenol, oligomeric reaction products with 1	500-655-7	161308-15-2	161308152	-	-	4826							-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
604-766-2	604-766-2	151006-58-5	151006585	-	-	4827	6.39	0.46	3	5.39	0.46		-4.7	-4.9	-6.3	0.00%	0.00%	0.00%
β-Alanine, N-(2-carboxyethyl)-, N-coco alkyl derivs., disodium sal	290-476-8	90170-43-7	90170437	-	-	4828	4.03	0.48	3	3.07	0.18		-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
613-583-7	613-583-7	64366-79-6	64366796	-	-	4829							-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
Fatty acids, C16-18 and C18-unsatd., Et esters	285-206-0	85049-36-1	85049361	-	-	4830							-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
Resin acids and Rosin acids, esters with diethylene glycol	268-884-2	68153-38-8	68153388	-	-	4831	6.33	0.45	3	5.33	0.45		-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
2,2-dimethyl-1,3-propanediyl dioleate	255-713-1	42222-50-4	42222504	-	-	4832	6.17	1.00	3	5.17	1.00		-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
Tar acids, 3,5-xylenol fraction	284-896-0	84989-07-1	84989071	-	-	4833	4.29	0.35	3	3.46	0.43		-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
628-862-9	628-862-9	1219458-11-3	1219458113	-	-	4834	2.16	0.70	3	1.16	0.70		-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
Decanol, branched and linear	291-169-1	90342-32-8	90342328	-	-	4835	3.44	0.24	3	2.44	0.24		-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
Nitric acid, reaction products with cyclododecanol and cyclodod	276-431-5	72162-23-3	72162233	-	-	4836							-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
3,4,5,5-tetramethylhex-2-ene	254-281-1	39083-38-0	39083380	-	-	4837							-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
614-270-8	614-270-8	68082-79-1	68082791	-	-	4838							-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
1,4-butanediylbis[oxy(2-hydroxy-3,1-propanediyl)] diacrylate	257-900-3	52408-42-1	52408421	-	-	4839	4.81		2				-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
Glycerides, C12-18 di- and tri-	294-590-9	91744-28-4	91744284	-	-	4840	4.54	0.33	3	3.54	0.33		-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
Resin acids and Rosin acids, maleated, esters with pentaerythrit	305-516-2	94581-17-6	94581176	-	-	4841							-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
605-293-4	605-293-4	162568-25-4	162568254	-	-	4842	5.38	0.22	3	4.38	0.22		-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
1,2-dichloro-1,1,2-trifluoro-2-(trifluoromethoxy)ethane	219-094-1	2356-53-8	2356538	-	-	4843							-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
1,2,4-Benzenetricarboxylic acid, tri-C9-11-alkyl esters	304-780-6	94279-36-4	94279364	-	-	4844	4.27	0.33	3	3.27	0.33		-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
Fatty acids, C16-18, lithium salts	272-195-2	68783-37-9	68783379	-	-	4845	5.52		3	4.52			-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
Fatty acids, C14-18 and C16-18-unsatd., esters with neopentyl gl	285-533-9	85116-81-0	85116810	-	-	4846	5.70	2.08	3	4.70	2.08		-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
β-Alanine, N-C8-18-alkyl derivs., monopotassium salts	290-475-2	90170-42-6	90170426	-	-	4847	4.79	0.78	3	3.79	0.78		-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
4,4'-Isopropylidenediphenol, polymer with 1-chloro-2,3-epoxypr	500-240-0	68958-77-0	68958770	-	-	4848							-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
Fatty acids, vegetable-oil, sulfated, sodium salts	262-996-5	61788-67-8	61788678	-	-	4849	5.43	0.55	3	4.43	0.55		-4.7	-5.0	-6.3	0.00%	0.00%	0.00%
zinc O,O,O',O'-tetrabutyl bis(phosphorodithioate)	230-257-6	6990-43-8	6990438	-	-	4850	4.19	0.61	3	3.19	0.61		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
Pentaerythritol, ethoxylated and propoxylated	500-069-1	30374-35-7	30374357	-	-	4851							-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
9-Octadecenoic acid (Z)-, reaction products with 2-[(2-aminoeth	272-379-2	68815-51-0	68815510	-	-	4852	5.51	0.32	3	4.51	0.32		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
Quaternary ammonium compounds, tri-C8-10-alkylmethyl, chlor	264-120-7	63393-96-4	63393964	-	-	4853	2.20	0.22	3	1.20	0.22		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
Benzene, ethylenated, by-products from	271-802-8	68608-82-2	68608822	-	-	4854	2.78	0.42	3	1.84	0.70		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
Amines, C16-22-alkyl	268-215-4	68037-92-3	68037923	-	-	4855	3.26	0.30	3	2.26	0.30		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
Fatty acids, C18-unsatd., reaction products with acrylic acid and	287-820-4	85586-18-1	85586181	-	-	4856	4.55	0.50	3	3.55	0.50		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
bis(tridecyl) adipate	241-029-0	16958-92-2	16958922	-	-	4857	6.68		1				-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
sodium N-methyl-N-(1-oxo-9-octadecenyl)aminoacetate	222-829-9	3624-77-9	3624779	-	-	4858	3.10	0.44	3	2.10	0.44		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
Phenol, dodecyl-, sulfurized, carbonates, calcium salts	272-233-8	68784-25-8	68784258	-	-	4859	6.07	0.42	3	5.07	0.42		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
Fatty acids, C14-18 and C16-18-unsatd., esters with propylene gl	284-864-6	84988-75-0	84988750	-	-	4860	4.57	1.07	3	3.57	1.07		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
629-767-5	629-767-5	1228186-18-2	1228186182	-	-	4861	2.36	0.49	3	1.36	0.49		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
800-309-8	800-309-8	231297-75-9	231297759	-	-	4862	6.50	0.45	3	5.50	0.45		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
Amines, (C16-18 and C18-unsatd. alkyl)dimethyl	268-220-1	68037-96-7	68037967	-	-	4863	2.12	0.66	3	1.18	0.77		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
Paraffin waxes and Hydrocarbon waxes, oxidized, lithium salts	272-032-5	68649-48-9	68649489	-	-	4864							-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
Fatty acids, C18-unsatd., dimers, methyl esters	500-225-9	68604-84-2	68604842	-	-	4865							-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
Fatty acids, C16-18, reaction products with diethanolamine	293-014-3	91032-08-5	91032085	-	-	4866	5.50		3	4.50			-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
Sorbitan monolaurate, ethoxylated	500-018-3	9005-64-5	9005645	-	-	4867	5.22	0.62	3	4.22	0.62		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
610-945-6	610-945-6	53037-34-6	53037346	-	-	4868	6.08	0.11	3	5.08	0.11		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
Fatty acids, lanolin, esters with pentaerythritol	270-434-5	68440-09-5	68440095	-	-	4869	5.12	0.98	3	4.12	0.98		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
N,N'-ethane-1,2-diylbisoleamide	203-756-1	110-31-6	110316	-	-	4870				2.68			-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
615-240-7	615-240-7	710292-85-6	710292856	-	-	4871	4.60	0.67	3	3.60	0.67		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
Amines, C12-14-tert-alkyl	273-279-1	68955-53-3	68955533	-	-	4872	3.04	0.34	3	1.90	0.60		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
sodium 4(or 5)-methyl-1H-benzotriazolide	265-004-9	64665-57-2	64665572	-	-	4873	4.87	0.44	3	3.59	0.57		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
isooctyl mercaptoacetate	246-613-9	25103-09-7	25103097	-	-	4874	3.14	0.47	3	2.22	0.63		-4.8	-5.0	-6.4	0.00%	0.00%	0.00%
orthoboric acid, compound with 2,2'-iminodiethanol	267-886-0	67952-33-4	67952334	-	-	4875	5.08	0.51	3	4.08	0.51		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
(octadecanoato-O)oxoaluminium	236-521-7	13419-15-3	13419153	-	-	4876	5.50		3	4.50			-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
dihydro-3-(octenyl)furan-2,5-dione	247-899-8	26680-54-6	26680546	-	-	4877	4.59		2				-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
Amines, C12-16-alkyldimethyl	270-414-6	68439-70-3	68439703	-	-	4878	2.36	0.66	4	1.18	0.77		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
Benzenesulfonic acid, mono-C11-13-branched alkyl derivs., sodi	271-808-0	68608-89-9	68608899	-	-	4879	3.90	0.35	3	2.90	0.35		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Fatty acids, C16-18, 2-octyldodecyl esters	306-232-1	96690-38-9	96690389	-	-	4880							-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
Cyclohexane, oxidized, distillates	308-380-2	97952-85-7	97952857	-	-	4881							-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
Resin acids and Rosin acids, fumarated, compds. with triethanol	293-625-5	91081-22-0	91081220	-	-	4882	4.42	2.07	3	3.42	2.07		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
N-octadecylstearamide	236-276-6	13276-08-9	13276089	-	-	4883							-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
Pyridine, alkyl derivs.	269-929-9	68391-11-7	68391117	-	-	4884	4.48	0.57	3	2.90	0.42		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
Cashew, nutshell liq., oligomeric reaction products with 1-chloro	500-210-7	68413-24-1	68413241	-	-	4885	5.50		3	4.50			-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
Rape oil, sulfated, ammonium salt	281-976-7	84082-28-0	84082280	-	-	4886	5.43	0.55	3	4.43	0.55		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
Glycerides, C16-18 mono-, di- and tri-	293-215-6	91052-54-9	91052549	-	-	4887	6.07	1.13	3	5.07	1.13		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
610-848-9	610-848-9	52479-58-0	52479580	-	-	4888	6.43	0.14	3	5.43	0.14		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
800-426-4	800-426-4	1373883-45-4	1373883454	-	-	4889	6.03	1.04	3	5.03	1.04		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
isooctadecan-1-ol	248-470-8	27458-93-1	27458931	-	-	4890	4.70	1.90	4	3.93	1.25		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
Fatty acids, C16-18, iso-Pr esters	292-962-5	91031-58-2	91031582	-	-	4891	6.16	1.16	3	5.16	1.16		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
isodecyl oleate	261-673-6	59231-34-4	59231344	-	-	4892	5.17	0.79	3	4.17	0.79		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
603-188-8	603-188-8	127184-53-6	127184536	-	-	4893							-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
Fatty acids, C16-18 and C18-unsatd., hexaesters with dipentaery	271-689-5	68604-38-6	68604386	-	-	4894				5.00			-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
Glycerides, mixed coco, decanoyl and octanoyl	271-729-1	68606-18-8	68606188	-	-	4895	5.37	0.30	3	4.37	0.30		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
676-712-6	676-712-6	68890-85-7	68890857	-	-	4896							-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
607-997-7	607-997-7	26776-30-7	26776307	-	-	4897							-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
4,4'-Isopropylidenediphenol, oligomeric reaction products with 1	500-302-7	113930-69-1	113930691	-	-	4898	4.55	0.94	3	3.55	0.94		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
1,2-Ethanediamine, N-(2-aminoethyl)-, reaction products with gl	291-221-3	90366-78-2	90366782	-	-	4899							-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
Alkenes, C15-18 α-, sulfurized	267-023-8	67762-55-4	67762554	-	-	4900	5.50		3	4.50			-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
607-907-6	607-907-6	26301-10-0	26301100	-	-	4901	6.04	0.81	3	5.04	0.81		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
isopropylnaphthalene	249-535-3	29253-36-9	29253369	-	-	4902	2.62	0.41	3	1.62	0.41		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
Peppermint, ext.	282-015-4	84082-70-2	84082702	-	-	4903	3.46	0.06	3	2.46			-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
Glycerides, C10-20 and C10-20-unsatd., oxidized	295-734-3	92128-40-0	92128400	-	-	4904	5.56	0.11	3	4.56	0.11		-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
2-Butenedioic acid (E)-, di-C12-18-alkyl esters	272-943-8	68921-51-7	68921517	-	-	4905	5.66		2				-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
Phosphoric acid, mono- and bis(branched and linear pentyl) este	282-784-6	84418-71-3	84418713	-	-	4906	5.05	0.33	3	4.05	0.33		-4.8	-5.1	-6.5	0.00%	0.00%	0.00%
Benzene-1,2,4-tricarboxylic acid 1,2-anhydride, oligomeric reacti	500-199-9	68183-39-1	68183391	-	-	4907							-4.8	-5.1	-6.5	0.00%	0.00%	0.00%
Fatty acids, tall-oil, reaction products with ethanolamine	270-445-5	68440-25-5	68440255	-	-	4908	3.75		1				-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Distillates (coal tar), naphthalene oils, methylnaphthalene fractic	309-985-4	101896-27-9	101896279	-	-	4909	4.01	0.88	3	3.01	1.11		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Fatty acids, C18-unsatd., dimers, hydrogenated, dimethyl esters	500-449-7	160901-12-2	160901122	-	-	4910							-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
605-315-2	605-315-2	163149-28-8	163149288	-	-	4911	6.64	0.29	3	5.64	0.29		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
614-560-4	614-560-4	68517-10-2	68517102	-	-	4912							-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, [[3-	279-767-0	81457-65-0	81457650	-	-	4913							-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
641-088-6	641-088-6	1229648-98-9	1229648989	-	-	4914	2.20	0.60	3	1.20	0.60		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
1,1-dimethylheptanethiol	246-896-9	25360-10-5	25360105	-	-	4915	2.43		1				-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
2-ethylhexanoic acid, monoester with propane-1,2-diol	285-503-5	85114-00-7	85114007	-	-	4916	4.43	0.25	3	3.43	0.25		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, [[3-	270-096-9	68411-04-1	68411041	-	-	4917							-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Fatty acids, C16-18, barium salts	292-883-6	91002-07-2	91002072	-	-	4918	5.42	0.57	3	3.80	0.22		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
(1-methylethyl)-1,1'-biphenyl	247-156-8	25640-78-2	25640782	-	-	4919	2.39	0.20	3	1.39	0.20		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Alcohols, C12-18, ethoxylated	500-201-8	68213-23-0	68213230	-	-	4920	2.81	0.37	3	1.81	0.37		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Reaction products of tall oil fatty acids with diethylenetriamine a	800-430-6	1419212-76-2	1419212762	-	-	4921							-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
1H-Imidazole-1-ethanol, 4,5-dihydro-, 2-nortall-oil alkyl derivs.	263-171-2	61791-39-7	61791397	-	-	4922	2.62	0.60	6	1.62	0.60		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
613-333-7	613-333-7	63705-03-3	63705033	-	-	4923	5.41	0.33	3	4.41	0.33		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Glycerides, C8-18	287-487-5	85536-06-7	85536067	-	-	4924	4.69	0.58	3	4.16	0.81		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Quaternary ammonium compounds, (C16-18 and C18-unsatd. al	268-074-9	68002-61-9	68002619	-	-	4925	1.97	0.47	3	0.97	0.47		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Sorbitan, (Z)-9-octadecenoate (2:3)	232-360-1	8007-43-0	8007430	-	-	4926	6.79	0.59	3	5.79	0.59		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
604-612-4	604-612-4	147900-93-4	147900934	-	-	4927	4.81	0.89	3	3.81	0.89		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
l-Glutamic acid, N-coco acyl derivs., disodium salts	269-085-1	68187-30-4	68187304	-	-	4928	4.84	0.30	3	3.84	0.30		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Glycerides, C16-18 mono-, di- and tri-, hydrogenated, citrates, sc	294-601-7	91744-39-7	91744397	-	-	4929	5.50		3	4.50			-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
4,4'-Isopropylidenediphenol, oligomeric reaction products with 1	500-090-6	36425-16-8	36425168	-	-	4930							-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Glycerides, palm-oil mono- and di-, hydrogenated	267-057-3	67784-87-6	67784876	-	-	4931	6.07	1.13	3	5.07	1.13		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Fatty acids, C16-18, iso-Bu esters	288-668-1	85865-69-6	85865696	-	-	4932	6.16	1.15	3	5.16	1.15		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Fatty acids, tall-oil, reaction products with pentaethylenehexami	288-927-9	85940-40-5	85940405	-	-	4933	3.44	0.20	3	2.70	0.40		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
1,3-dihydro-4(or 5)-methyl-2H-benzimidazole-2-thione, zinc salt	262-872-0	61617-00-3	61617003	-	-	4934	3.60	0.37	3	2.87	1.48		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Fatty acids, C14-18 and C18-unsatd., branched and linear, Me es	286-065-8	85186-80-7	85186807	-	-	4935							-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Pyridinium, 1-(phenylmethyl)-, ethyl methyl derivs., chlorides	272-695-0	68909-18-2	68909182	-	-	4936	3.41	1.10	3	2.41	1.10		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
Fatty acids, C16-18 and C18-unsatd., esters with pentaerythritol	288-305-7	85711-45-1	85711451	-	-	4937	4.90	0.72	3	3.90	0.72		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
628-863-4	628-863-4	1219458-14-6	1219458146	-	-	4938	2.27	0.61	3	1.60	0.66		-4.9	-5.1	-6.5	0.00%	0.00%	0.00%
1,3-Cyclohexanedimethanamine	219-941-5	2579-20-6	2579206	-	-	4939	4.82	0.23	3	4.11	0.28		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Reaction products of coconut oil with polyethyleneglycol and 2-e	640-964-5	218451-68-4	218451684	-	-	4940	4.64	0.39	3	3.70	0.40		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Nitriles, C16-22	268-861-7	68153-02-6	68153026	-	-	4941							-4.9	-5.2	-6.5	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Amides, tall-oil fatty, N,N-di-Me	269-665-4	68308-74-7	68308747	-	-	4942	3.43	0.52	3	2.47	0.46		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Ethanesulfonic acid, 2-(methylamino)-, N-coco acyl derivs., sodiu	263-174-9	61791-42-2	61791422	-	-	4943	4.11	0.50	3	3.11	0.50		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Alcohols, C12-18, ethoxylated, sulfates, sodium salts	500-189-4	68081-91-4	68081914	-	-	4944	3.96	0.50	3	2.96	0.50		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
629-735-0	629-735-0	1226892-50-7	1226892507	-	-	4945	2.90	0.58	3	1.90	0.58		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Fatty acids, C18-unsatd., dimers, oligomeric reaction products w	500-382-3	157707-73-8	157707738	-	-	4946	3.88	0.34	3	2.94	0.41		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
612-396-8	612-396-8	61791-19-3	61791193	-	-	4947	3.50	0.38	3	2.70	0.41		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Phosphonic acid, mixed C12-20-alkyl and C14-18-unsatd. alkyl de	300-326-6	93925-25-8	93925258	-	-	4948	5.50		3	4.50			-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
N,N''-methylenebis[N'-[3-(hydroxymethyl)-2,5-dioxoimidazolidin	254-372-6	39236-46-9	39236469	-	-	4949	4.71	0.67	3	3.71	0.67		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
2-ethylhexyl diphenyl phosphite	239-716-5	15647-08-2	15647082	-	-	4950							-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu a	273-527-9	68988-45-4	68988454	-	-	4951	3.73	0.50	3	2.78	0.61		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
[tetrachloro-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]co	248-573-8	27614-71-7	27614717	-	-	4952	5.40		2	3.00			-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, bro	270-958-4	68512-13-0	68512130	-	-	4953	5.40		2	3.00			-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
629-720-9	629-720-9	1219826-66-0	1219826660	-	-	4954	2.43	0.68	3	1.57	0.61		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
800-182-9	800-182-9	1426148-68-6	1426148686	-	-	4955	5.19	0.27	3	4.19	0.27		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
609-530-2	609-530-2	38172-91-7	38172917	-	-	4956	5.66		1				-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
isodecyl pivalate	262-108-6	60209-82-7	60209827	-	-	4957	4.78		1	3.30			-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Reaction products of ethane-1,2-diol and 1,2-epoxybutane	695-757-2	897381-19-0	897381190	-	-	4958							-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Aluminum, benzoate C16-18-fatty acids complexes	303-385-6	94166-87-7	94166877	-	-	4959	5.50		3	4.50			-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Quaternary ammonium compounds, C12-18-alkylbis(hydroxyeth	276-038-9	71808-53-2	71808532	-	-	4960	3.07	0.93	3	2.50	0.98		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Terpenes and terpenoids, turpentine-oil, α-pinene fraction, oligo	500-245-8	70750-57-1	70750571	-	-	4961	2.73	0.31	3	1.73	0.31		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
pentasodium pentahydrogen [[(phosphonatomethyl)imino]bis[e	263-212-4	61792-09-4	61792094	-	-	4962	5.41	1.21	3	4.39	1.46		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Isooctadecanoic acid, reaction products with tetraethylenepenta	272-225-4	68784-17-8	68784178	-	-	4963	5.45	1.30	3	4.45	1.30		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Lipase, triacylglycerol	232-619-9	9001-62-1	9001621	-	-	4964	5.17	0.54	3	4.17	0.54		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Quaternary ammonium compounds, benzyl-C12-16-alkyldimeth	270-325-2	68424-85-1	68424851	-	-	4965	2.84	0.61	22	1.84	0.61	22	-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Fatty acids, C16-18 and C18-unsatd., iso-Bu esters	284-868-8	84988-79-4	84988794	-	-	4966	6.00	1.18	3	5.00	1.18		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Tetra-n-butyl titanate, polymer with water	500-687-1	162303-51-7	162303517	-	-	4967	6.00	0.33	3	5.00	0.33		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
695-101-5	695-101-5	1275611-65-8	1275611658	-	-	4968							-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Cocoa, powd., alkalized	305-748-4	95009-22-6	95009226	-	-	4969	4.47		1				-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Fatty acids, C16-18, 2-hexyldecyl esters	309-832-1	101227-09-2	101227092	-	-	4970	6.50	1.00	3	5.50	1.00		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Fatty acids, C6-18, 2,2-dimethyl-1,3-propanediyl esters	292-927-4	91031-27-5	91031275	-	-	4971	6.17	1.00	3	5.17	1.00		-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
696-364-9	696-364-9	133779-11-0	133779110	-	-	4972	2.05	0.51	3	1.05	0.51		-4.9	-5.2	-6.6	0.00%	0.00%	0.00%
600-026-8	600-026-8	1000817-22-0	1000817220	-	-	4973	3.63	0.40	3	2.85	0.36		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
isopropyl isodecanoate	269-023-3	68171-33-5	68171335	-	-	4974	5.24		1	5.00			-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
pentaerythritol tetraoleate	242-960-5	19321-40-5	19321405	-	-	4975	5.25	0.75	3	4.25	0.75		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
616-248-3	616-248-3	75627-31-5	75627315	-	-	4976	3.46	0.28	3	2.83	0.37		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Glycerides, C14-18 mono- and di-	266-952-6	67701-33-1	67701331	-	-	4977	6.07	1.13	3	5.07	1.13		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Titanium, diethylene glycol propylene glycol triethanolamine cor	272-250-0	68784-48-5	68784485	-	-	4978	5.75	1.24	3	4.75	1.24		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
oleic acid, compound with N-(2-aminoethyl)ethane-1,2-diamine	241-924-6	18016-43-8	18016438	-	-	4979	3.98	0.49	3	3.05	0.40		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	219-514-3	2451-62-9	2451629	-	-	4980	4.47		1				-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Octadecanoic acid, 12-hydroxy-, reaction products with ethylene	309-629-8	100545-48-0	100545480	-	-	4981							-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
2,3-dihydroxypropyl 12-hydroxyoctadecanoate	228-507-4	6284-43-1	6284431	-	-	4982	6.07	0.97	3	5.07	0.97		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
692-946-1	692-946-1	649747-80-8	649747808	-	-	4983	5.64	0.99	3	4.64	0.99		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
696-028-1	696-028-1	1334537-35-7	1334537357	-	-	4984							-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Reaction mass of ammonium 4-amino-3-nitrobenzenesulfonate	700-384-6	82324-60-5	82324605	-	-	4985							-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
614-587-1	614-587-1	68551-92-8	68551928	-	-	4986	5.50		3	4.50			-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
4,4'-Methylenediphenyl diisocyanate, oligomeric reaction produ	500-297-1	109331-54-6	109331546	-	-	4987	3.98		1	4.00			-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Mannanase, endo-1,4-β-	253-446-5	37288-54-3	37288543	-	-	4988	5.17	0.34	3	4.17	0.34		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Soybean oil, epoxidized, reaction products with methanol	287-837-7	85586-35-2	85586352	-	-	4989	5.27	0.40	3	4.27	0.40		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Fatty acids, tallow, calcium salts	265-228-7	64755-01-7	64755017	-	-	4990	5.74	1.14	3	4.74	1.14		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
sodium glucoheptonate	250-480-2	31138-65-5	31138655	-	-	4991	6.08	0.75	3	5.08	0.75		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Phosphoric acid, butyl ester	235-826-2	12788-93-1	12788931	-	-	4992	5.04	0.13	3	4.45	0.17		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
608-744-3	608-744-3	32472-85-8	32472858	-	-	4993	5.45	0.12	3	4.45	0.12		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Glycerides, mixed C8-10 and succinyl	294-620-0	91744-56-8	91744568	-	-	4994	5.15	0.60	3	4.15	0.60		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
614-339-2	614-339-2	68154-62-1	68154621	-	-	4995	3.67	0.22	3	3.01	0.31		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Tall oil, potassium salt	271-968-1	68647-71-2	68647712	-	-	4996	5.28	1.67	3	3.88	1.03		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Fatty acids, C14-18 and C18-unsatd., branched and linear, esters	284-957-1	85005-25-0	85005250	-	-	4997	4.24		1	2.32			-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Resin acids and Rosin acids, esters with ethylene glycol	270-986-7	68512-65-2	68512652	-	-	4998	6.20	0.63	3	5.20	0.63		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Sorbitan, isooctadecanoate	276-171-2	71902-01-7	71902017	-	-	4999				4.20			-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
610-559-8	610-559-8	50658-23-6	50658236	-	-	5000				4.00			-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Phosphoric acid, hexyl ester	270-935-9	68511-03-5	68511035	-	-	5001							-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
monoethanolamine oleate	218-878-0	2272-11-9	2272119	-	-	5002	4.58	1.09	3	3.79	1.14		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Heptanoic acid, ester with 2-ethyl-2-(hydroxymethyl)-1,3-propar	267-029-0	67762-64-5	67762645	-	-	5003	5.91	0.75	3	4.91	0.75		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%

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Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
800-029-6	800-029-6	1290049-56-7	1290049567	-	-	5004	2.29	0.16	3	1.29	0.16		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Amines, C36-alkylenedi-	273-282-8	68955-56-6	68955566	-	-	5005	3.67	1.58	3	2.67	1.58		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
1,2,3-Propanetriol, glycidyl ethers	292-011-4	90529-77-4	90529774	-	-	5006	5.24	1.71	3	4.24	1.71		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Quaternary ammonium compounds, bis(hydrogenated tallow all	263-090-2	61789-80-8	61789808	-	-	5007	3.14	0.40	3	2.14	0.40		-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
3-(2-dodecenyl)succinic anhydride	243-296-9	19780-11-1	19780111	-	-	5008	4.59		2				-5.0	-5.2	-6.6	0.00%	0.00%	0.00%
Sorbitan, octanoate (2:3)	295-118-4	91844-53-0	91844530	-	-	5009	4.80	0.73	3	3.80	0.73		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
606-712-3	606-712-3	211450-54-3	211450543	-	-	5010	4.58	0.55	3	3.58	0.55		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
608-035-9	608-035-9	27014-42-2	27014422	-	-	5011							-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
1,3-Propanediamine, N-[3-(tridecyloxy)propyl]-, branched	270-851-2	68479-04-9	68479049	-	-	5012	2.72		1				-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
Fatty acids, C8-10, zinc salts	293-048-9	91051-00-2	91051002	-	-	5013	2.44	0.40	3	1.89	0.67		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
mono- and di-esterification products of propane-1,2,3-triol and f	800-149-9	1410795-90-2	1410795902	-	-	5014	5.48	1.01	3	4.48	1.01		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
Resin acids and Rosin acids, hydrogenated, Me esters	232-476-2	8050-15-5	8050155	-	-	5015	6.20	0.63	3	5.20	0.63		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
1-[1,3-bis(hydroxymethyl)-2,5-dioxoimidazolidin-4-yl]-1,3-bis(hy	278-928-2	78491-02-8	78491028	-	-	5016	4.59	0.52	4	3.94	0.61		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
806-508-6	806-508-6	1419212-77-3	1419212773	-	-	5017							-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
tetradonium bromide	214-291-9	1119-97-7	1119977	-	-	5018	2.57	1.33	4	0.95	1.25		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
609-542-8	609-542-8	383178-66-3	383178663	-	-	5019	4.10	0.35	3	3.21	0.27		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
Tar bases, coal, picoline fraction	295-548-2	92062-33-4	92062334	-	-	5020							-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
800-760-0	800-760-0	68139-89-9	68139899	-	-	5021	4.85		2				-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
Phenol, heptyl derivs.	276-743-1	72624-02-3	72624023	-	-	5022	2.89	0.46	3	1.89	0.80		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
2-Butenedioic acid (E)-, di-C8-18-alkyl esters	271-880-3	68610-90-2	68610902	-	-	5023	5.66		2				-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
1,3,5-Triazine-2,4,6-triamine, deammoniated	272-034-6	68649-66-1	68649661	-	-	5024							-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
Formaldehyde, reaction products with ethylenediamine	281-928-5	84066-92-2	84066922	-	-	5025	4.83	0.78	3	3.83	0.78		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
Fatty acids, C16-18, tetraesters with 3,3'-oxybis[1,2-propanediol	293-026-9	91050-80-5	91050805	-	-	5026	6.87	0.37	3	5.87	0.37		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
Fatty acids, tall-oil, iron salts	263-009-0	61788-81-6	61788816	-	-	5027							-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
609-271-5	609-271-5	36609-29-7	36609297	-	-	5028	5.18	0.30	3	4.23	0.28		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
Isooctadecanoic acid, mono- and diesters with glycerol	306-657-2	97358-80-0	97358800	-	-	5029	6.07	0.97	3	5.07	0.97		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
3-(methacryloylamino)-N,N-dimethylpropan-1-aminium 4-(C10-1	688-489-2	1024700-50-2	1024700502	-	-	5030	4.46		2	3.05			-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
611-591-5	611-591-5	57903-73-8	57903738	-	-	5031	4.47	0.85	3	3.47	0.85		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
Fatty acids, C8-10, mixed esters with adipic acid and trimethylol	306-085-3	95912-89-3	95912893	-	-	5032							-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
Decanoic acid, mixed esters with neopentyl glycol and octanoic a	274-764-0	70693-32-2	70693322	-	-	5033	4.01	1.93	3	3.01	1.93		-5.0	-5.3	-6.6	0.00%	0.00%	0.00%
benzene-1,2,4,5-tetracarboxylic acid, compound with 4,5-dihydr	259-224-4	54553-90-1	54553901	-	-	5034	4.96	1.28	3	3.96	1.28		-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
Propanenitrile, 3,3'-iminobis-, N-tallow alkyl derivs.	270-194-1	68412-52-2	68412522	-	-	5035							-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
1-(tert-dodecylthio)propan-2-ol	266-582-5	67124-09-8	67124098	-	-	5036	3.96	1.05	3	2.96	1.05		-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
613-868-6	613-868-6	65997-12-8	65997128	-	-	5037	6.20	0.63	3	5.20	0.63		-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
2-octyldodecyl isooctadecanoate	298-361-4	93803-87-3	93803873	-	-	5038							-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
Alcohols, C8-10, ethoxylated, sulfates, ammonium salts	500-233-2	68891-29-2	68891292	-	-	5039	4.65	0.43	3	3.65	0.43		-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
Glycerides, C8-10 mono- and di-	287-488-0	85536-07-8	85536078	-	-	5040	4.88	0.33	3	4.18	0.66		-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
2-Hexyldecan-1-ol, ethoxylated	500-116-6	52609-19-5	52609195	-	-	5041	3.20	0.51	3	1.90	0.44		-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
613-584-2	613-584-2	64401-02-1	64401021	-	-	5042	3.78		1				-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
2,4,7,9-Tetramethyldec-5-yne-4,7-diol, ethoxylated	500-022-5	9014-85-1	9014851	-	-	5043	4.60	0.37	3	3.50	0.73		-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
Rape oil, reaction products with diethanolamine	269-125-8	68187-80-4	68187804	-	-	5044	3.78	0.53	3	2.68	0.28		-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
638-747-5	638-747-5	1228186-17-1	1228186171	-	-	5045	3.14	0.40	3	2.14	0.40		-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
604-714-9	604-714-9	149968-48-9	149968489	-	-	5046	3.13		2				-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
oleic acid, monoester with oxybis(propanediol)	256-367-4	49553-76-6	49553766	-	-	5047	3.20		2	3.38			-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
zinc bis[O-(2-ethylhexyl)] bis[O-(isobutyl)] bis(dithiophosphate)	247-810-2	26566-95-0	26566950	-	-	5048	4.84	0.77	3	3.84	0.77		-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
Fatty acids, C18-unsatd., dimers, oligomeric reaction products w	500-289-8	103758-98-1	103758981	-	-	5049	3.68	0.20	3	2.93	0.42		-5.1	-5.3	-6.7	0.00%	0.00%	0.00%
604-617-1	604-617-1	147993-66-6	147993666	-	-	5050	3.59	0.82	3	2.59	0.82		-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
Poly(oxy-1,2-ethanediyl),α-hydro-ω-hydroxy- Ethane-1,2-diol, et	500-038-2	25322-68-3	25322683	-	-	5051	6.48	0.79	7	5.48	0.79		-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
dioctyltin dilaurate	222-883-3	3648-18-8	3648188	-	-	5052	3.91	0.76	3	2.91	0.76		-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-3-en-2-one	265-450-4	65113-95-3	65113953	-	-	5053	3.63	0.50	3	2.79	0.53		-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
Hydrocarbons, C12-30, olefin-rich, ethylene polymn. by-product	272-762-4	68911-05-7	68911057	-	-	5054	3.32	1.28	3	3.84	2.11		-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
DL-lysine monohydrochloride	200-739-0	70-53-1	70531	-	-	5055							-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
800-310-3	800-310-3	78683-74-6	78683746	-	-	5056							-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
Alcohols, lanolin, distn. residues	292-441-2	90622-40-5	90622405	-	-	5057							-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
806-509-1	806-509-1	1393571-42-0	1393571420	-	-	5058							-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
Polysulfides, di-tert-nonyl	270-336-2	68425-16-1	68425161	-	-	5059	3.22	1.61	3	2.22	1.61		-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
Phosphoric acid, mixed esters with Bu alc. and ethylene glycol	284-716-0	84962-20-9	84962209	-	-	5060	5.04	0.13	3	4.45	0.17		-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
2,3-Epoxypropyl neodecanoate, oligomeric reaction products wi	500-281-4	98362-33-5	98362335	-	-	5061	4.42		1				-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
Glycerides, C14-18 and C16-18-unsatd. mono-, di- and tri-	293-187-5	91052-28-7	91052287	-	-	5062	5.47		1	4.00			-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
Benzenamine, reaction products with aniline hydrochloride and	309-913-1	101357-16-8	101357168	-	-	5063	3.35	0.42	3	2.35	0.42		-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
4,4'-Isopropylidenediphenol, oligomeric reaction products with 1	500-652-0	161308-12-9	161308129	-	-	5064	3.30		1				-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
600-028-9	600-028-9	1001254-87-0	1001254870	-	-	5065							-5.1	-5.4	-6.7	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Fatty acids, lanolin, iso-Pr esters	264-119-1	63393-93-1	63393931	-	-	5066	5.64	0.88	3	4.64	0.88		-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
sorbitan tristearate	247-891-4	26658-19-5	26658195	-	-	5067				4.20			-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
Formaldehyde, reaction products with m-phenylenediamine, soc	274-986-8	70892-34-1	70892341	-	-	5068	5.30	0.25	3	4.30	0.25		-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
Resin acids and Rosin acids, maleated, calcium salts	294-402-5	91722-01-9	91722019	-	-	5069	4.20	0.27	3	4.18	0.78		-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
Quaternary ammonium compounds, (hydrogenated tallow alkyl)	263-005-9	61788-78-1	61788781	-	-	5070	1.97	0.64	3	1.27	0.63		-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
Butanedioic acid, sulfo-, monoesters with lanolin alcs., disodium	290-844-8	90268-43-2	90268432	-	-	5071	5.07	0.92	3	4.07	0.92		-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
Butanedioic acid, sulfo-, 4-[2-[(2-hydroxyethyl)amino]ethyl] este	308-072-8	97862-28-7	97862287	-	-	5072	4.21	0.36	3	3.21	0.36		-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
Fatty acids, C14-18 and C16-18-unsatd., mixed esters with casto	295-653-3	92113-48-9	92113489	-	-	5073				5.04			-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
800-906-3	800-906-3	1402434-48-3	1402434483	-	-	5074	1.71		2				-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
Phosphoric acid, mono- and di-C12-14-alkyl esters	308-020-4	97808-97-4	97808974	-	-	5075							-5.1	-5.4	-6.7	0.00%	0.00%	0.00%
800-362-7	800-362-7	1307863-78-0	1307863780	-	-	5076	3.28	0.59	3	2.28	0.59		-5.1	-5.4	-6.8	0.00%	0.00%	0.00%
9-Octadecenoic acid (Z)-, isooctyl ester, reaction products with g	306-111-3	96152-40-8	96152408	-	-	5077	5.23	0.58	3	4.45	0.54		-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
Fatty acids, tall-oil, magnesium salts	266-942-1	67701-23-9	67701239	-	-	5078							-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
2-Propenoic acid, 2-methyl-, 2-hydroxyethyl ester, phosphate	258-053-2	52628-03-2	52628032	-	-	5079	4.85		1				-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
2-Butenedioic acid (E)-, di-C16-18-alkyl esters	272-944-3	68921-52-8	68921528	-	-	5080	5.66		2				-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-ol	267-140-4	67801-20-1	67801201	-	-	5081	3.63	0.50	3	2.79	0.53		-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
Peptones, beef	293-426-3	91079-38-8	91079388	-	-	5082							-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
menthane, monohydroperoxy derivative	247-987-6	26762-92-5	26762925	-	-	5083	3.79	0.37	3	3.14	0.43		-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
695-121-4	695-121-4	1178870-70-6	1178870706	-	-	5084							-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
800-767-9	800-767-9	1424148-94-6	1424148946	-	-	5085	4.33	0.82	3	3.33	0.82		-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
zinc bis[bis(dodecylphenyl)] bis(dithiophosphate)	259-048-8	54261-67-5	54261675	-	-	5086	4.11	0.74	3	4.02	1.08		-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
Sulfonium compounds, C11-14-alkylbis(hydroxyethyl), 2-hydroxy	278-855-6	78169-20-7	78169207	-	-	5087	2.69	1.29	3	1.69	1.29		-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
dihydro-3-(tripropenyl)furan-2,5-dione	295-556-6	92077-08-2	92077082	-	-	5088				4.69			-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
fatty acids, C16-18 and C18-unsatd., isooctyl esters, epoxidized	307-159-8	97553-05-4	97553054	-	-	5089	5.99	0.85	3	4.99	0.85		-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
Hexafluoropropene, oxidized, oligomers, reduced, fluorinated	500-537-5	161075-00-9	161075009	-	-	5090	3.60	2.13	3	2.60	2.13		-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
605-658-8	605-658-8	173011-06-8	173011068	-	-	5091	4.38	0.75	3	3.38	0.75		-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
3-methyl-5-phenylpentanol	259-461-3	55066-48-3	55066483	-	-	5092	4.18	0.12	3	3.52	0.15		-5.2	-5.4	-6.8	0.00%	0.00%	0.00%
isodecyl acrylate	215-542-5	1330-61-6	1330616	-	-	5093	3.29	0.18	3	2.35	0.21		-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
604-250-7	604-250-7	141773-73-1	141773731	-	-	5094	3.41	0.28	3	2.45	0.23		-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
(octahydro-4,7-methano-1H-indenediyl)bis(methylene) diacrylat	255-901-3	42594-17-2	42594172	-	-	5095	3.31		2				-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
Rape oil, sulfated, sodium salt	281-978-8	84082-30-4	84082304	-	-	5096	4.74	0.51	3	3.74	0.51		-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
Amines, N-C16-22-alkyltrimethylenedi-	292-564-1	90640-45-2	90640452	-	-	5097	3.00	1.90	3	2.00	1.90		-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
Dodecan-1-ol, ethoxylated	500-002-6	9002-92-0	9002920	-	-	5098	3.52	0.30	13	2.52	0.30	13	-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
[N,N,N',N',N'',N''-hexaethyl-29H,31H-phthalocyaninetrimethylan	249-125-4	28654-73-1	28654731	-	-	5099							-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
N,N-dibutyloleamide	227-410-4	5831-80-1	5831801	-	-	5100							-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
614-482-0	614-482-0	68439-46-3	68439463	-	-	5101	3.54	0.38	3	2.54	0.38		-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
800-153-0	800-153-0	1313206-64-2	1313206642	-	-	5102	2.76	0.54	3	1.76	0.54		-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
3-(methacryloylamino)-N,N,N-trimethylpropan-1-aminium 4-(C1	688-159-8	1024699-81-7	1024699817	-	-	5103	3.94		2	3.05			-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
695-088-6	695-088-6	135458-18-3	135458183	-	-	5104							-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
613-645-3	613-645-3	646505-36-4	646505364	-	-	5105	5.35	0.29	3	4.35	0.29		-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
Aluminum, hydrobis(2-methylpropyl)-, reaction products with is	274-261-6	70024-64-5	70024645	-	-	5106							-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
di(isooctadecanoic) acid, diester with oxydi(propanediol)	267-821-6	67938-21-0	67938210	-	-	5107	5.33	0.67	3	4.33	0.67		-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
696-481-5	696-481-5	1219826-47-7	1219826477	-	-	5108	1.25		1				-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
isooctyl 3-mercaptopropionate	250-157-6	30374-01-7	30374017	-	-	5109	2.14	0.64	3	1.20	0.46		-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
1,1,3,3-tetramethylbutyl peroxyneodecanoate	257-077-0	51240-95-0	51240950	-	-	5110	5.30		1				-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
2,2-bis(hydroxymethyl)-1,3-propanediyl dioleate	246-665-2	25151-96-6	25151966	-	-	5111	6.17	0.89	3	5.17	0.89		-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
600-687-2	600-687-2	105839-18-7	105839187	-	-	5112	2.73	0.47	3	1.73	0.47		-5.2	-5.5	-6.8	0.00%	0.00%	0.00%
619-721-2	619-721-2	1079258-99-3	1079258993	-	-	5113							-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
2,6-dimethylindan-1-amine	937-760-6	1225478-65-8	1225478658	-	-	5114							-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
Reaction mass of ammonium 2-amino-4-[(4-amino-6-chloro-1,3,!	937-657-6	1362924-06-8	1362924068	-	-	5115							-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
800-766-3	800-766-3	1424148-97-9	1424148979	-	-	5116	4.33	0.82	3	3.33	0.82		-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
800-765-8	800-765-8	1424149-03-0	1424149030	-	-	5117	4.68	0.57	3	3.68	0.57		-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
Reaction mass of dimethyl 2,2,4-trimethylhexanedioate and dim	700-087-1	201872-72-2	201872722	-	-	5118	5.28		2				-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
607-104-0	607-104-0	225375-65-5	225375655	-	-	5119	6.58		1				-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
O,O-bis(methylphenyl) hydrogen dithiophosphate	248-273-7	27157-94-4	27157944	-	-	5120							-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
nonene	248-339-5	27215-95-8	27215958	-	-	5121							-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
(1R*,6S*)-6-(ethoxycarbonyl)-N,N-dimethyl-6-phenylcyclohex-2-	700-689-4	41524-32-7	41524327	-	-	5122	4.50		1				-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
3,7-dimethylnona-2,6-dienenitrile	263-214-5	61792-11-8	61792118	-	-	5123	3.42	0.22	3	2.42	0.22		-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
Extract oils (coal), tar base	266-020-9	65996-86-3	65996863	-	-	5124							-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
Butanal, reaction products with aniline	270-109-8	68411-20-1	68411201	-	-	5125	4.53	0.56	3	3.53	0.56		-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
Gases (petroleum), acetylene manuf. off	270-745-6	68477-64-5	68477645	-	-	5126							-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
Urea, reaction products with formaldehyde	271-898-1	68611-64-3	68611643	-	-	5127	4.85		1				-5.2	-5.5	-6.9	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Propanenitrile, 3-amino-, N-coco alkyl derivs.	272-244-8	68784-40-7	68784407	-	-	5128	2.52		1				-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
6,10-dimethylundeca-5,9-dien-2-one	211-711-2	689-67-8	689678	-	-	5129	3.83		1				-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
Coconut oil, hydrogenated	284-283-8	84836-98-6	84836986	-	-	5130							-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
distillates (coal tar), upper, fluorene-rich	284-900-0	84989-11-7	84989117	-	-	5131							-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
Amines, N-(3-aminopropyl)-N-tallow alkyltrimethylenedi-	288-048-0	85632-63-9	85632639	-	-	5132	2.11		1				-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
isohexadecene	288-853-7	85909-49-5	85909495	-	-	5133							-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
Alkyl iodides, C6-18, perfluoro	292-474-2	90622-71-2	90622712	-	-	5134							-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
Fatty acids, C18-22	292-772-2	90990-11-7	90990117	-	-	5135				3.60			-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
dodecahydro-3a,6,6,9a-tetramethylnaphtho[2,1-b]furan	223-118-6	3738-00-9	3738009	-	-	5136	3.54	0.29	3	2.54	0.29		-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
Fatty acids, coco, isotridecyl esters	292-997-6	91031-91-3	91031913	-	-	5137	3.14	2.96	3	2.14	2.96		-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
607-255-2	607-255-2	236391-76-7	236391767	-	-	5138	3.76	0.35	3	2.76	0.35		-5.2	-5.5	-6.9	0.00%	0.00%	0.00%
613-848-7	613-848-7	65870-94-2	65870942	-	-	5139	5.78	0.44	3	4.78	0.44		-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
Glycerides, C12-18 mono- and di-	293-209-3	91052-49-2	91052492	-	-	5140	4.54	0.33	3	3.54	0.33		-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
614-255-6	614-255-6	68071-07-8	68071078	-	-	5141	3.78	0.57	3	2.78	0.57		-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
695-977-9	695-977-9	1309955-79-0	1309955790	-	-	5142	2.55	0.48	3	1.55	0.48		-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
614-452-7	614-452-7	68410-23-1	68410231	-	-	5143	3.75	0.11	3	3.03	0.28		-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
Fatty acids, C14-18 and C16-18-unsatd., isotridecyl esters	285-541-2	85116-88-7	85116887	-	-	5144	5.17	0.79	3	4.17	0.79		-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
Alkenes, C24-28 α-	300-203-7	93924-11-9	93924119	-	-	5145	3.32	1.28	3	3.84	2.11		-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
Lysozyme (chicken egg white)	235-747-3	12650-88-3	12650883	-	-	5146							-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
Alcohols, C16-18, ethoxylated, phosphates	500-295-0	106233-09-4	106233094	-	-	5147	3.37	0.62	3	2.37	0.62		-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
2-Butenedioic acid (E)-, di-C18-22-alkyl esters	272-945-9	68921-53-9	68921539	-	-	5148							-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
Fatty acids, tall-oil, reaction products with boric acid (H3BO3) an	294-785-9	91770-03-5	91770035	-	-	5149	5.43	1.10	3	4.43	1.10		-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
Fatty acids, C8-10, triesters with trimethylolpropane	293-036-3	91050-89-4	91050894	-	-	5150	6.28	0.87	3	5.28	0.87		-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
Amines, tri-C8-10-alkyl	272-347-8	68814-95-9	68814959	-	-	5151	3.20	1.03	5	2.20	1.03		-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
Phosphoric acid, isononyl ester	284-851-5	84988-61-4	84988614	-	-	5152	5.17	0.48	3	4.35	0.27		-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
627-071-6	627-071-6	1233873-37-4	1233873374	-	-	5153	3.98	1.28	3	2.98	1.28		-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
Hydrochloric acid, reaction products with aniline and nitrobenze	291-454-0	90411-76-0	90411760	-	-	5154	5.23	0.45	3	4.23	0.45		-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
Decanoic acid, mixed esters with heptanoic acid, octanoic acid, p	275-118-0	71010-76-9	71010769	-	-	5155							-5.3	-5.5	-6.9	0.00%	0.00%	0.00%
608-711-3	608-711-3	32167-31-0	32167310	-	-	5156	4.73		2				-5.3	-5.6	-6.9	0.00%	0.00%	0.00%
Tall oil, compd. with ethanolamine	268-069-1	68002-54-0	68002540	-	-	5157	4.56	0.95	3	3.32	1.07		-5.3	-5.6	-6.9	0.00%	0.00%	0.00%
Propylidynetrimethanol, ethoxylated, esters with acrylic acid, re	500-425-6	159034-91-0	159034910	-	-	5158	4.49		1				-5.3	-5.6	-6.9	0.00%	0.00%	0.00%
Naphthenic acids, potassium salts	266-120-2	66072-08-0	66072080	-	-	5159	3.75	0.72	3	2.75	0.72		-5.3	-5.6	-6.9	0.00%	0.00%	0.00%
Tall oil, compd. with diethanolamine	268-452-3	68092-28-4	68092284	-	-	5160	4.69	1.32	3	3.79	0.61		-5.3	-5.6	-6.9	0.00%	0.00%	0.00%
Alcohols, C12-15, ethoxylated	500-195-7	68131-39-5	68131395	-	-	5161	3.05	0.47	6	2.46	0.39		-5.3	-5.6	-6.9	0.00%	0.00%	0.00%
614-557-8	614-557-8	68515-81-1	68515811	-	-	5162	3.94	0.38	3	2.94	0.38		-5.3	-5.6	-6.9	0.00%	0.00%	0.00%
[N,N,N',N',N'',N''-hexaethyl-29H,31H-phthalocyaninetrimethylan	278-150-3	75247-18-6	75247186	-	-	5163	4.56		1				-5.3	-5.6	-6.9	0.00%	0.00%	0.00%
630-459-8	630-459-8	1225197-81-8	1225197818	-	-	5164	2.93	0.57	3	2.30	0.24		-5.3	-5.6	-6.9	0.00%	0.00%	0.00%
Cyclohexane, oxidized, non-volatile residue	270-147-5	68411-76-7	68411767	-	-	5165	5.47	0.37	3	4.47	0.37		-5.3	-5.6	-6.9	0.00%	0.00%	0.00%
806-914-3	806-914-3	1499182-59-0	1499182590	-	-	5166							-5.3	-5.6	-6.9	0.00%	0.00%	0.00%
Asphalt, sulfonated, sodium salt	269-212-0	68201-32-1	68201321	-	-	5167	6.48	1.15	3	4.91	0.36		-5.3	-5.6	-6.9	0.00%	0.00%	0.00%
N-[9-(dichloromethylidene)-1,2,3,4-tetrahydro-1,4-methanonapl	691-719-4	1072957-71-1	1072957711	-	-	5168	1.88	0.73	3	1.33	0.98		-5.3	-5.6	-7.0	0.00%	0.00%	0.00%
methyl 3,5,5-trimethylhexanoate	807-032-1	71500-39-5	71500395	-	-	5169							-5.3	-5.6	-7.0	0.00%	0.00%	0.00%
Sorbitan monostearate, ethoxylated	500-020-4	9005-67-8	9005678	-	-	5170	5.12	0.32	4	4.12	0.32		-5.3	-5.6	-7.0	0.00%	0.00%	0.00%
Myristica fragrans, ext.	282-013-3	84082-68-8	84082688	-	-	5171	3.84		2				-5.4	-5.6	-7.0	0.00%	0.00%	0.00%
triisononanoic acid, triester with 2,2'-[oxybis(methylene)]bis[2-(h	270-560-0	68443-84-5	68443845	-	-	5172							-5.4	-5.6	-7.0	0.00%	0.00%	0.00%
Benzoic acid, 2-hydroxy-, mono-C>13-alkyl derivs., calcium salts	281-018-8	83846-43-9	83846439	-	-	5173							-5.4	-5.6	-7.0	0.00%	0.00%	0.00%
Reaction mass of bis[2,4-bis(2-methylbutan-2-yl)phenyl] 4-(2-me	700-485-5	939402-02-5	939402025	-	-	5174	5.42	0.15	3	4.42	0.15		-5.4	-5.7	-7.0	0.00%	0.00%	0.00%
Phosphoric acid, mono- and di-C6-10-alkyl esters	269-616-7	68307-94-8	68307948	-	-	5175	4.75	1.09	3	3.75	1.09		-5.4	-5.7	-7.0	0.00%	0.00%	0.00%
mercaptoacetic acid, monoester with propane-1,2,3-triol	250-264-8	30618-84-9	30618849	-	-	5176	4.15	0.36	3	3.03	0.39		-5.4	-5.7	-7.0	0.00%	0.00%	0.00%
800-770-5	800-770-5	1424148-99-1	1424148991	-	-	5177	4.28	0.69	3	3.28	0.69		-5.4	-5.7	-7.0	0.00%	0.00%	0.00%
607-234-8	607-234-8	234446-82-3	234446823	-	-	5178	5.48	0.43	3	4.24	0.53		-5.4	-5.7	-7.0	0.00%	0.00%	0.00%
Resin acids and Rosin acids, hydrogenated, esters with triethyler	271-996-4	68648-53-3	68648533	-	-	5179	6.20	0.63	3	5.20	0.63		-5.4	-5.7	-7.0	0.00%	0.00%	0.00%
605-694-4	605-694-4	173832-46-7	173832467	-	-	5180							-5.4	-5.7	-7.1	0.00%	0.00%	0.00%
Ammonium difluoro{[2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,	682-238-0	1190931-27-1	1190931271	-	-	5181	5.63	0.37	3	4.63	0.37		-5.5	-5.7	-7.1	0.00%	0.00%	0.00%
pentan-2-one O-(4,10-dimethyl-7-vinyl-6,8-dioxa-5,9-diaza-7-sila	700-810-0	58190-62-8	58190628	-	-	5182	5.37	0.27	3	4.37	0.27		-5.5	-5.7	-7.1	0.00%	0.00%	0.00%
Octadecanoic acid, reaction products with diethylenetriamine ar	284-698-4	84962-05-0	84962050	-	-	5183	3.28	2.38	3	2.28	2.38		-5.5	-5.7	-7.1	0.00%	0.00%	0.00%
5-isopropylimidazolidine-2,4-dione	634-107-4	16935-34-5	16935345	-	-	5184							-5.5	-5.7	-7.1	0.00%	0.00%	0.00%
5-methyl-2-(1-methylvinyl)cyclohexan-1-ol	232-102-8	7786-67-6	7786676	-	-	5185	4.73		1				-5.5	-5.7	-7.1	0.00%	0.00%	0.00%
diisotridecyl 3,3'-[(dibutylstannylene)bis(thio)]dipropionate	284-461-5	84896-44-6	84896446	-	-	5186	3.30	0.92	3	2.60	0.28		-5.5	-5.7	-7.1	0.00%	0.00%	0.00%
Heptadecanol, branched and linear	291-378-8	90388-00-4	90388004	-	-	5187	4.83	1.15	3	3.83	1.15		-5.5	-5.7	-7.1	0.00%	0.00%	0.00%
2-Butene, chlorinated, epoxidized, distn. residues	304-783-2	94279-39-7	94279397	-	-	5188							-5.5	-5.7	-7.1	0.00%	0.00%	0.00%
1-Propene, 2-methyl-, chlorinated, epoxidized, distn. residues	304-801-9	94279-55-7	94279557	-	-	5189							-5.5	-5.7	-7.1	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
2-ethyl-2-[[(1-oxoisooctadecyl)oxy]methyl]-1,3-propanediyl bis(i	271-347-5	68541-50-4	68541504	-	-	5190				5.04			-5.5	-5.8	-7.1	0.00%	0.00%	0.00%
Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]	272-732-0	68910-13-4	68910134	-	-	5191	5.26	1.21	3	4.26	1.21		-5.6	-5.9	-7.2	0.00%	0.00%	0.00%
Tar bases, coal, lutidine fraction	293-766-2	91082-52-9	91082529	-	-	5192							-5.6	-5.9	-7.2	0.00%	0.00%	0.00%
tris(dodecyl and/or octyl) benzene-1,2,4-tricarboxylate	700-342-7	1163775-81-2	1163775812	-	-	5193	4.14	0.31	3	3.14	0.31		-5.6	-5.9	-7.2	0.00%	0.00%	0.00%
dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione	254-100-6	38720-66-0	38720660	-	-	5194	5.18	0.72	3	4.18	0.72		-5.7	-5.9	-7.3	0.00%	0.00%	0.00%
reaction products of zinc oxide and glycerol	700-107-9	87189-25-1	87189251	-	-	5195							-5.7	-5.9	-7.3	0.00%	0.00%	0.00%
Esterification product of castor oil and tetrahydromethyl-1,3-isol	700-064-6	1059667-42-3	1059667423	-	-	5196							-5.7	-5.9	-7.3	0.00%	0.00%	0.00%
Coupling reaction products of diazotized 2-amino-6-[(2-sulfoeth	700-470-3	1198102-85-0	1198102850	-	-	5197	5.29	0.36	3	4.29	0.36		-5.7	-6.0	-7.3	0.00%	0.00%	0.00%
Resin acids and Rosin acids, reaction products with formaldehyd	696-130-6	1364681-45-7	1364681457	-	-	5198	5.83	0.58	3	4.83	0.58		-5.7	-6.0	-7.3	0.00%	0.00%	0.00%
Ethyl-2-cyano-2-ethyl-3-methylhexanoate	700-063-0	100453-11-0	100453110	-	-	5199							-5.8	-6.1	-7.4	0.00%	0.00%	0.00%
D-Glucopyranose, oligomers, branched and linear C9-11-alkyl gly	500-394-9	157707-87-4	157707874	-	-	5200	4.00	0.67	3	3.00	0.67		-5.8	-6.1	-7.4	0.00%	0.00%	0.00%
Resin acids and Rosin acids, Me esters	269-035-9	68186-14-1	68186141	-	-	5201	6.20	0.63	3	5.20	0.63		-5.9	-6.1	-7.5	0.00%	0.00%	0.00%
Potassium difluoro{[2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-	682-240-1	1190931-39-5	1190931395	-	-	5202	5.63	0.37	3	4.63	0.37		-5.9	-6.2	-7.5	0.00%	0.00%	0.00%
Reaction products of 2,2'-oxydiethanol and 3-(triethoxysilyl)prop	688-124-7	152261-43-3	152261433	-	-	5203							-5.9	-6.2	-7.5	0.00%	0.00%	0.00%
7,7,9(or 7,9,9)-trimethyl-4,13-dioxo-3,14-dioxa-5,12-diazahexad	276-957-5	72869-86-4	72869864	-	-	5204							-5.9	-6.2	-7.5	0.00%	0.00%	0.00%
dibutyltin bis(2-ethylhexanoate)	220-481-2	2781-10-4	2781104	-	-	5205	3.04	0.28	3	2.04	0.28		-6.0	-6.2	-7.6	0.00%	0.00%	0.00%
Reaction products of diazotized 5-({4-[(3-amino-4-sulfophenyl)ar	619-894-4	958872-41-8	958872418	-	-	5206							-6.0	-6.2	-7.6	0.00%	0.00%	0.00%
Difluoro{[2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4	682-239-6	1190931-41-9	1190931419	-	-	5207	5.63	0.37	3	4.63	0.37		-6.0	-6.3	-7.6	0.00%	0.00%	0.00%
Silicic acid (H4SiO4), tetraethyl ester, reaction products with bis(	300-344-4	93925-42-9	93925429	-	-	5208	3.25	1.39	3	2.25	1.39		-6.0	-6.3	-7.6	0.00%	0.00%	0.00%
D-Glucopyranose, oligomeric, C10-16 (even numbered) alkyl glyc	664-492-4	742087-49-6	742087496	-	-	5209	4.58		2				-6.0	-6.3	-7.6	0.00%	0.00%	0.00%
606-441-0	606-441-0	201305-16-0	201305160	-	-	5210							-6.0	-6.3	-7.7	0.00%	0.00%	0.00%
Esterification products of 2,2'-(oxydimethanediyl)bis[2-(hydroxy	700-325-4	1149346-12-2	1149346122	-	-	5211	5.27	1.23	3	4.27	1.23		-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
Reaction mass of (2R,2'R)-2'-methylspiro[4-azoniabicyclo[2.2.2]c	696-667-6	1292815-90-7	1292815907	-	-	5212							-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
3-(6-chloro-5-fluoropyrimidin-4-yl)-2-(2,4-difluorophenyl)-1-(1H-	639-694-0	188416-20-8	188416208	-	-	5213							-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
Tetradecan- l-ol, ethoxylated	500-059-7	27306-79-2	27306792	-	-	5214							-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
1-Methoxy-3-pentadecylbenzene-[29H,31H-phthalocyaninato(2-	700-057-8	350600-52-1	350600521	-	-	5215	5.00		1				-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
D-Glucopyranose, oligomeric, decyl octyl glucosides, phosphinic	664-495-0	740817-98-5	740817985	-	-	5216	4.74	0.31	3	3.74	0.31		-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
619-566-0	619-566-0	848301-65-5	848301655	-	-	5217	3.88		2				-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
619-567-6	619-567-6	848301-66-6	848301666	-	-	5218	4.79	1.20	3	3.79	1.20		-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
619-568-1	619-568-1	848301-67-7	848301677	-	-	5219	6.20	0.54	3	5.20	0.54		-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
Reaction mass of abieta-8,11,13-trien-18-yl [(5-{[(abieta-8,11,13-	700-056-2	934985-96-3	934985963	-	-	5220							-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
Esterification product of polypropylene glycol ether with glycero	700-332-2	935442-45-8	935442458	-	-	5221							-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
Reaction products of Hydrogenated C18-unsaturated fatty acid c	700-271-1	943862-64-4	943862644	-	-	5222							-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
Ethyl 3-(2,4-dimethyl-1,3-dioxolan-2-yl)propanoate	700-636-5	5413-49-0	5413490	-	-	5223	5.65		1				-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
Ethyl 3-[4-(hydroxymethyl)-2-methyl-1,3-dioxolan-2-yl]propanoa	700-637-0	902272-78-0	902272780	-	-	5224	5.59		1				-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
Reaction products of chlorosulfonated reaction products of copp	696-533-7	1025071-45-7	1025071457	-	-	5225	4.96		1				-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
5',5'''-{(phenylmethanediyl)bis[(2-methoxybenzene-4,1-diyl)diaz	700-136-7	1062263-18-6	1062263186	-	-	5226	3.40	1.38	3	2.44	1.12		-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
1,1'-ethan-1,2-diylbisbenzene, brominated	700-158-7	1092834-40-6	1092834406	-	-	5227							-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
700-772-5	700-772-5	1190961-28-4	1190961284	-	-	5228							-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
hydroxylamines, di-C16-18 (even numbered) alkyl	801-599-9	1374859-51-4	1374859514	-	-	5229							-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
esterification products of castor oil and polyphosphoric acids	614-406-6	68308-61-2	68308612	-	-	5230	5.27	0.31	3	4.27	0.31		-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
Reaction products of racemic lactic acid, partially neutralized wit	700-937-1	1312021-45-6	1312021456	-	-	5231	4.54		1				-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
3-(C6-16, (even numbered) and C16 unsaturated alkyl)-4-(C7-17	700-132-5	863782-35-8	863782358	-	-	5232							-6.1	-6.3	-7.7	0.00%	0.00%	0.00%
Coupling reaction products of 3,3'-dichlorobiphenyl-4,4'-bis(diaz	700-452-5	1032192-65-6	1032192656	-	-	5233							-6.1	-6.4	-7.7	0.00%	0.00%	0.00%
Coupling reaction products of 3,3'-dichlorobiphenyl-4,4'-bis(diaz	700-448-3	1032192-78-1	1032192781	-	-	5234							-6.1	-6.4	-7.7	0.00%	0.00%	0.00%
tris[2-(4,4-dimethylpentan-2-yl)-5,7,7-trimethyloctyl] 2-hydroxyp	700-590-6	56727-25-4	56727254	-	-	5235	2.68		2				-6.1	-6.4	-7.7	0.00%	0.00%	0.00%
4,4'-methanediylbis(2,6-dimethylcyclohexanamine)	634-657-5	65962-45-0	65962450	-	-	5236	4.03	0.63	3	3.19	0.83		-6.1	-6.4	-7.7	0.00%	0.00%	0.00%
C13-(branched)-alkyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propic	700-397-7	847488-62-4	847488624	-	-	5237							-6.1	-6.4	-7.7	0.00%	0.00%	0.00%
3-[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]propane-1,2-diol	289-296-2	87061-04-9	87061049	-	-	5238	5.00		2				-6.1	-6.4	-7.7	0.00%	0.00%	0.00%
benzene-1,2,4,5-tetracarboxylic acid, compound with 4,5-dihydr	259-226-5	54553-91-2	54553912	-	-	5239	4.28	1.26	3	3.28	1.26		-6.1	-6.4	-7.7	0.00%	0.00%	0.00%
9-hydroxy-5,9-dimethyldec-4-enal	940-437-2	926-50-1	926501	-	-	5240	4.81		1				-6.2	-6.4	-7.8	0.00%	0.00%	0.00%
2,2-di(tetrahydrofuryl)propane	700-263-8	89686-69-1	89686691	-	-	5241							-6.2	-6.4	-7.8	0.00%	0.00%	0.00%
2-(acetylamino)-N-benzyl-3-methoxypropanamide	700-539-8	175481-26-2	175481262	-	-	5242							-6.2	-6.5	-7.9	0.00%	0.00%	0.00%
reaction products of 1,6-diisocyanatohexane with 2-[(2-methacr	700-151-9	1101874-33-2	1101874332	-	-	5243							-6.3	-6.5	-7.9	0.00%	0.00%	0.00%
619-816-9	619-816-9	128446-33-3	128446333	-	-	5244	5.50		3	4.50			-6.3	-6.6	-7.9	0.00%	0.00%	0.00%
ethyl 2-allyl-2-cyano-3-methylhexanoate	700-062-5	33422-23-0	33422230	-	-	5245							-6.3	-6.6	-7.9	0.00%	0.00%	0.00%
2,7-naphthalenedisulfonic acid, 4-amino-5-hydroxy-, diazotized,	232-380-0	8011-86-7	8011867	-	-	5246	3.89	1.03	3	2.89	1.03		-6.3	-6.6	-7.9	0.00%	0.00%	0.00%
Reaction mass of benzyl 2-(2-methoxyethoxy)ethyl adipate and l	940-202-4	1175612-76-6	1175612766	-	-	5247	4.29		1				-6.4	-6.6	-8.0	0.00%	0.00%	0.00%
Reaction products of 3-(trimethoxysilyl)propane-1-thiol and 5-isc	700-534-0	117172-56-2	117172562	-	-	5248	4.97		1				-6.4	-6.7	-8.0	0.00%	0.00%	0.00%
[2,9,16,23-tetrachloro-29H,31H-phthalocyaninato(2-)-N29,N30,N	240-183-6	16040-69-0	16040690	-	-	5249	5.40		2	3.00			-6.5	-6.7	-8.1	0.00%	0.00%	0.00%
N-benzyl-2-bromo-3-methoxypropanamide	700-538-2	705283-58-5	705283585	-	-	5250							-6.5	-6.7	-8.1	0.00%	0.00%	0.00%
Alkanes, C10-13-iso-	271-366-9	68551-17-7	68551177	-	-	5251	6.42	0.32	3	5.42	0.32		-6.5	-6.8	-8.1	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]		TP(Cwcoast) [-]
tetrahydro-6-(3-pentenyl)-2H-pyran-2-one	251-201-7	32764-98-0	32764980	-	-	5252	4.49		1				-6.5	-6.8	-8.1	0.00%	0.00%		0.00%
5-cyclohexyl-2-methylpentan-1-ol	700-146-1	1141487-54-8	1141487548	-	-	5253	3.05	0.28	3	2.09	0.37		-6.6	-6.9	-8.2	0.00%	0.00%		0.00%
691-736-7	691-736-7	960495-42-5	960495425	-	-	5254							-6.7	-6.9	-8.3	0.00%	0.00%		0.00%
Reaction products of N-(1-oxododecyl)-L-glutamic acid and 2-oct	700-285-8	1034015-52-5	1034015525	-	-	5255							-6.7	-6.9	-8.3	0.00%	0.00%		0.00%
Esterification products of N-Methyl-N-(1-oxotetradecyl)-β-alanin	700-369-4	1085852-72-7	1085852727	-	-	5256							-6.7	-6.9	-8.3	0.00%	0.00%		0.00%
614-947-8	614-947-8	693217-63-9	693217639	-	-	5257	5.00		1				-6.7	-7.0	-8.3	0.00%	0.00%		0.00%
N,N-diisopropyl-3-(2-methoxy-5-methylphenyl)-3-phenylpropan	700-655-9	857288-56-3	857288563	-	-	5258	3.00		2				-6.7	-7.0	-8.3	0.00%	0.00%		0.00%
ethyl 3-amino-3-phenylpropanoate	613-206-6	6335-76-8	6335768	-	-	5259							-6.9	-7.1	-8.5	0.00%	0.00%		0.00%
Reaction products of chlorosulfonated reaction products of copp	802-101-2	1246273-07-3	1246273073	-	-	5260							-6.9	-7.1	-8.5	0.00%	0.00%		0.00%
Reaction products of L-lysine and N-[(3S)-2,6-dioxotetrahydro-2	688-011-2	1243654-79-6	1243654796	-	-	5261	4.45	0.38	3	3.45	0.38		-6.9	-7.1	-8.5	0.00%	0.00%		0.00%
6-[(2-{[5-({3-methyl-2,7-dioxo-1-[(3-sulfophenyl)carbonyl]-2,7-dil	700-450-4	1007553-30-1	1007553301	-	-	5262							-6.9	-7.1	-8.5	0.00%	0.00%		0.00%
Reaction products of chlorosulfonated reaction products of copp	700-449-9	1007578-75-7	1007578757	-	-	5263	5.83	0.58	3	4.83	0.58		-6.9	-7.1	-8.5	0.00%	0.00%		0.00%
N,N'-bis[2-hydroxy-3-(2,2,3,3-tetrafluoropropoxy)propyl]-N,N,N',	700-737-4	1220100-43-5	1220100435	-	-	5264	3.51		2				-6.9	-7.1	-8.5	0.00%	0.00%		0.00%
700-904-1	700-904-1	1350725-68-6	1350725686	-	-	5265	5.30	0.34	3	4.30	0.34		-6.9	-7.1	-8.5	0.00%	0.00%		0.00%
2-{[2,2,4-trifluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}eth	700-535-6	1190931-34-0	1190931340	-	-	5266							-7.0	-7.2	-8.6	0.00%	0.00%		0.00%
N-palmitoylisoleucine	627-025-5	101541-04-2	101541042	-	-	5267							-7.2	-7.5	-8.8	0.00%	0.00%		0.00%
3-(4-isobutylcyclohexyl)propanal	940-042-5	1254940-85-6	1254940856	-	-	5268	3.59		2				-7.2	-7.5	-8.8	0.00%	0.00%		0.00%
Pentadecanol, branched and linear	291-807-9	90480-71-0	90480710	-	-	5269				1.39			-7.6	-7.9	-9.2	0.00%	0.00%		0.00%
3-(hexyloxy)propane-1,2-diol	600-386-6	10305-38-1	10305381	-	-	5270							-8.5	-8.8	-10.1	0.00%	0.00%		0.00%
REACH - petroleum (not on SOLUTIONS' MLoS)																			
count							*306*	*301*	*306*	*304*	*301*	*0*	*326*	*326*	*326*	*326*	*326*	*11.3%*	*326*
sum																*1.0%*	*1.7%*	*88.6%*	*0.001%*
standard deviation							*1.14*	*0.38*		*1.076*	*0.46*		*1.2*	*1.2*	*1.2*				
2.5-p													*-8.1*	*-7.9*	*-9.9*	*2.2E-16*	*1.7E-15*		*3.2E-23*
50-p							*4.16*	*0.54*	*3*	*3.41*	*0.60*		*-5.3*	*-5.1*	*-7.0*	*5.7E-08*	*2.2E-07*		*1.0E-12*
97.5-p													*-3.5*	*-3.2*	*-5.2*	*2.4E-04*	*5.9E-04*		*8.8E-08*
Fuels, diesel	269-822-7	68334-30-5	68334305	-	-	5272	4.32	0.58	3	3.55	0.52		-2.9	-2.7	-4.6	0.20%	0.34%	0.34%	0.00%
Fuel oil, residual	270-675-6	68476-33-5	68476335	-	-	5273	4.16	0.98	3	3.46	1.41		-3.1	-2.9	-4.9	0.09%	0.20%	0.53%	0.00%
Gasoline	289-220-8	86290-81-5	86290815	-	-	5274	4.13	0.46	3	3.13	0.46		-3.2	-2.9	-4.9	0.08%	0.19%	0.72%	0.00%
Kerosine (petroleum)	232-366-4	8008-20-6	8008206	-	-	5275	4.01	0.65	3	3.01	0.67		-3.4	-3.1	-5.1	0.04%	0.09%	0.81%	0.00%
Residues (petroleum), atmospheric	269-777-3	68333-22-2	68333222	-	-	5276	4.16	0.98	3	3.46	1.41		-3.5	-3.2	-5.2	0.03%	0.07%	0.87%	0.00%
Residues (petroleum), atm. tower	265-045-2	64741-45-3	64741453	-	-	5277	4.16	0.98	3	3.46	1.41		-3.5	-3.2	-5.2	0.03%	0.07%	0.94%	0.00%
Distillates (petroleum), full-range straight-run middle	272-341-5	68814-87-9	68814879	-	-	5278	4.26	0.61	3	3.59	0.60		-3.5	-3.2	-5.2	0.02%	0.06%	1.00%	0.00%
Gas oils (petroleum), heavy vacuum	265-058-3	64741-57-7	64741577	-	-	5279	4.16	0.98	3	3.46	1.41		-3.5	-3.2	-5.2	0.02%	0.06%	1.06%	0.00%
Naphtha (petroleum), full-range straight-run	265-042-6	64741-42-0	64741420	-	-	5280	4.13	0.46	3	3.13	0.46		-3.5	-3.2	-5.2	0.02%	0.06%	1.12%	0.00%
Residues (petroleum), vacuum	265-057-8	64741-56-6	64741566	-	-	5281							-3.5	-3.3	-5.3	0.02%	0.05%	1.16%	0.00%
Kerosine (petroleum), hydrodesulfurized	265-184-9	64742-81-0	64742810	-	-	5282	4.01	0.65	3	3.01	0.67		-3.6	-3.3	-5.3	0.02%	0.05%	1.21%	0.00%
Distillates (petroleum), hydrodesulfurized middle	265-183-3	64742-80-9	64742809	-	-	5283	4.25	0.61	3	3.59	0.60		-3.6	-3.3	-5.3	0.02%	0.05%	1.26%	0.00%
Distillates (petroleum), vacuum	274-685-1	70592-78-8	70592788	-	-	5284	4.16	0.98	3	3.46	1.41		-3.8	-3.5	-5.5	0.01%	0.02%	1.28%	0.00%
Kerosine (petroleum), sweetened	294-799-5	91770-15-9	91770159	-	-	5285	4.01	0.65	3	3.01	0.67		-3.8	-3.5	-5.5	0.01%	0.02%	1.30%	0.00%
Gas oils (petroleum), light vacuum	265-059-9	64741-58-8	64741588	-	-	5286	4.28	0.58	3	3.55	0.52		-3.8	-3.6	-5.5	0.01%	0.02%	1.32%	0.00%
Naphtha (petroleum), catalytic reformed	273-271-8	68955-35-1	68955351	-	-	5287	4.13	0.46	3	3.13	0.46		-3.8	-3.6	-5.6	0.01%	0.02%	1.33%	0.00%
Distillates (petroleum), petroleum residues vacuum	273-263-4	68955-27-1	68955271	-	-	5288	4.16	0.98	3	3.46	1.41		-3.9	-3.6	-5.6	0.01%	0.02%	1.35%	0.00%
Gas oils (petroleum), straight-run	265-043-1	64741-43-1	64741431	-	-	5289	4.26	0.60	3	3.59	0.59		-3.9	-3.6	-5.6	0.01%	0.02%	1.36%	0.00%
Asphalt	232-490-9	8052-42-4	8052424	-	-	5290							-3.9	-3.6	-5.6	0.01%	0.01%	1.38%	0.00%
Distillates (petroleum), light catalytic cracked	265-060-4	64741-59-9	64741599	-	-	5291	2.68	0.62	3	1.68	0.62		-3.9	-3.6	-5.6	0.01%	0.01%	1.39%	0.00%
Residues (petroleum), thermal cracked	265-081-9	64741-80-6	64741806	-	-	5292	4.16	0.98	3	3.46	1.41		-3.9	-3.6	-5.6	0.01%	0.01%	1.41%	0.00%
Naphtha (petroleum), full-range reformed	272-895-8	68919-37-9	68919379	-	-	5293	4.13	0.46	3	3.13	0.46		-3.9	-3.7	-5.6	0.00%	0.01%	1.42%	0.00%
Naphtha (petroleum), light catalytic cracked	265-056-2	64741-55-5	64741555	-	-	5294	4.13	0.46	3	3.13	0.46		-3.9	-3.7	-5.6	0.00%	0.01%	1.43%	0.00%
Naphtha (petroleum), light straight-run	265-046-8	64741-46-4	64741464	-	-	5295	4.09	0.45	3	3.09	0.45		-3.9	-3.7	-5.7	0.00%	0.01%	1.44%	0.00%
Naphtha (petroleum), hydrodesulfurized light	265-178-6	64742-73-0	64742730	-	-	5296	4.13	0.46	3	3.13	0.46		-4.0	-3.7	-5.7	0.00%	0.01%	1.45%	0.00%
Fuels, diesel, no. 2	270-676-1	68476-34-6	68476346	-	-	5297	4.28	0.58	3	3.55	0.52		-4.0	-3.7	-5.7	0.00%	0.01%	1.46%	0.00%
Naphtha (petroleum), heavy straight-run	265-041-0	64741-41-9	64741419	-	-	5298	4.13	0.46	3	3.13	0.46		-4.0	-3.7	-5.7	0.00%	0.01%	1.47%	0.00%
Residues (petroleum), hydrocracked	265-076-1	64741-75-9	64741759	-	-	5299	4.16	0.97	3	3.46	1.38		-4.0	-3.8	-5.7	0.00%	0.01%	1.48%	0.00%
Lubricating oils	278-012-2	74869-22-0	74869220	-	-	5300	6.29	1.09	3	5.29	1.09		-4.0	-3.8	-5.8	0.00%	0.01%	1.49%	0.00%
Gas oils (petroleum), hydrodesulfurized heavy vacuum	265-189-6	64742-86-5	64742865	-	-	5301	4.16	0.98	3	3.46	1.41		-4.0	-3.8	-5.8	0.00%	0.01%	1.50%	0.00%
Naphtha (petroleum), hydrotreated heavy	265-150-3	64742-48-9	64742489	-	-	5302	4.13	0.46	3	3.13	0.46		-4.0	-3.8	-5.8	0.00%	0.01%	1.50%	0.00%
Distillates (petroleum), hydrotreated middle	265-148-2	64742-46-7	64742467	-	-	5303	4.25	0.61	3	3.59	0.60		-4.1	-3.8	-5.8	0.00%	0.01%	1.51%	0.00%
Gas oils (petroleum), hydrodesulfurized	265-182-8	64742-79-6	64742796	-	-	5304	4.25	0.61	3	3.59	0.60		-4.1	-3.8	-5.8	0.00%	0.01%	1.52%	0.00%
Naphtha (petroleum), isomerization	265-073-5	64741-70-4	64741704	-	-	5305	4.13	0.46	3	3.13	0.46		-4.1	-3.9	-5.8	0.00%	0.01%	1.52%	0.00%
Naphtha (petroleum), light catalytic cracked sweetened	295-441-0	92045-59-5	92045595	-	-	5306	4.13	0.46	3	3.13	0.46		-4.2	-3.9	-5.9	0.00%	0.00%	1.53%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION					EXPECTED IMPACT in 'EU WATER'						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [·]	Z(Cwfresh) [·]	Z(Cwcoast) [·]	TP(Cwlocal) [-]	TP(Cwfresh) [-]		TP(Cwcoast) [-]
Naphtha (petroleum), heavy catalytic cracked	265-055-7	64741-54-4	64741544	-	-	5307	4.13	0.46	3	3.13	0.46		-4.2	-3.9	-5.9	0.00%	0.00%	1.53%	0.00%
Distillates (petroleum), light hydrocracked	265-078-2	64741-77-1	64741771	-	-	5308	4.28	0.58	3	3.55	0.52		-4.2	-3.9	-5.9	0.00%	0.00%	1.54%	0.00%
Naphtha (petroleum), heavy catalytic reformed	265-070-9	64741-68-0	64741680	-	-	5309	4.13	0.46	3	3.13	0.46		-4.2	-4.0	-5.9	0.00%	0.00%		0.00%
Residues (petroleum), thermal cracked vacuum	295-518-9	92062-05-0	92062050	-	-	5310							-4.2	-4.0	-5.9	0.00%	0.00%		0.00%
Naphtha (petroleum), light catalytic reformed	265-065-1	64741-63-5	64741635	-	-	5311	4.13	0.46	3	3.13	0.46		-4.2	-4.0	-5.9	0.00%	0.00%		0.00%
Distillates (petroleum), heavy straight-run	272-817-2	68915-96-8	68915968	-	-	5312	4.26	0.61	3	3.59	0.60		-4.2	-4.0	-6.0	0.00%	0.00%		0.00%
Distillates (petroleum), straight-run middle	265-044-7	64741-44-2	64741442	-	-	5313	4.26	0.61	3	3.59	0.60		-4.2	-4.0	-6.0	0.00%	0.00%		0.00%
Distillates (petroleum), light thermal cracked	265-084-5	64741-82-8	64741828	-	-	5314	2.68	0.62	3	1.68	0.62		-4.2	-4.0	-6.0	0.00%	0.00%		0.00%
Naphtha (petroleum), hydrotreated light	265-151-9	64742-49-0	64742490	-	-	5315	4.12	0.44	3	3.12	0.44		-4.2	-4.0	-6.0	0.00%	0.00%		0.00%
Residues (petroleum), catalytic cracking	295-511-0	92061-97-7	92061977	-	-	5316	4.16	0.98	3	3.46	1.41		-4.3	-4.0	-6.0	0.00%	0.00%		0.00%
Naphtha (petroleum), unsweetened	272-186-3	68783-12-0	68783120	-	-	5317	4.13	0.46	3	3.13	0.46		-4.3	-4.0	-6.0	0.00%	0.00%		0.00%
Naphtha (petroleum), sweetened	265-089-2	64741-87-3	64741873	-	-	5318	4.13	0.46	3	3.13	0.46		-4.3	-4.0	-6.0	0.00%	0.00%		0.00%
Distillates (petroleum), heavy paraffinic	265-052-0	64741-51-1	64741511	-	-	5319	4.83	2.06	3	3.83	2.06		-4.3	-4.1	-6.0	0.00%	0.00%		0.00%
Fuel oil, no. 6	271-384-7	68553-00-4	68553004	-	-	5320	4.16	0.98	3	3.46	1.41		-4.3	-4.1	-6.0	0.00%	0.00%		0.00%
Naphtha (petroleum), full-range alkylate, butane-contg.	271-267-0	68527-27-5	68527275	-	-	5321	4.13	0.46	3	3.13	0.46		-4.4	-4.1	-6.1	0.00%	0.00%		0.00%
Naphtha (petroleum), hydrodesulfurized full-range	295-433-7	92045-52-8	92045528	-	-	5322	4.13	0.46	3	3.13	0.46		-4.4	-4.1	-6.1	0.00%	0.00%		0.00%
Distillates (petroleum), heavy hydrocracked	265-077-7	64741-76-0	64741760	-	-	5323	6.29	1.09	3	5.29	1.09		-4.4	-4.1	-6.1	0.00%	0.00%		0.00%
Asphalt, oxidized	265-196-4	64742-93-4	64742934	-	-	5324							-4.4	-4.1	-6.1	0.00%	0.00%		0.00%
Fuel oil, no. 2	270-671-4	68476-30-2	68476302	-	-	5325	4.28	0.58	3	3.55	0.51		-4.4	-4.1	-6.1	0.00%	0.00%		0.00%
Distillates (petroleum), hydrodesulfurized light catalytic cracked	269-781-5	68333-25-5	68333255	-	-	5326	2.68	0.61	3	1.68	0.61		-4.4	-4.1	-6.1	0.00%	0.00%		0.00%
Gas oils (petroleum), hydrotreated vacuum	265-162-9	64742-59-2	64742592	-	-	5327	4.16	0.98	3	3.46	1.41		-4.4	-4.1	-6.1	0.00%	0.00%		0.00%
Distillates (petroleum), light vacuum	274-684-6	70592-77-7	70592777	-	-	5328	4.16	0.98	3	3.46	1.41		-4.4	-4.1	-6.1	0.00%	0.00%		0.00%
Naphtha (petroleum), sweetened light	309-976-5	101795-01-1	101795011	-	-	5329	4.13	0.46	3	3.13	0.46		-4.4	-4.2	-6.1	0.00%	0.00%		0.00%
Distillates (petroleum), solvent-dewaxed heavy paraffinic	265-169-7	64742-65-0	64742650	-	-	5330	6.29	1.07	3	5.29	1.07		-4.4	-4.2	-6.2	0.00%	0.00%		0.00%
Naphtha (petroleum), hydrodesulfurized heavy	265-185-4	64742-82-1	64742821	-	-	5331	4.13	0.46	3	3.13	0.46		-4.4	-4.2	-6.2	0.00%	0.00%		0.00%
Residues (petroleum), vacuum, light	292-658-2	90669-76-4	90669764	-	-	5332	4.16	0.98	3	3.46	1.41		-4.4	-4.2	-6.2	0.00%	0.00%		0.00%
Hydrocarbons, C4, ethylene-manuf.-by-product	270-691-3	68476-52-8	68476528	-	-	5333	4.19	0.23	3	3.19	0.23		-4.5	-4.2	-6.2	0.00%	0.00%		0.00%
Fuel gases	270-667-2	68476-26-6	68476266	-	-	5334	4.41	0.39	3	3.41	0.39		-4.5	-4.2	-6.2	0.00%	0.00%		0.00%
xylene	215-535-7	1330-20-7	1330207	-	-	5335	4.59	0.70	20	3.59	0.70		-4.5	-4.2	-6.2	0.00%	0.00%		0.00%
Gasoline, pyrolysis, debutanizer bottoms	271-726-5	68606-10-0	68606100	-	-	5336	3.30	0.22	3	2.30	0.22		-4.5	-4.2	-6.2	0.00%	0.00%		0.00%
Distillates (petroleum), intermediate vacuum	274-683-0	70592-76-6	70592766	-	-	5337	4.16	0.98	3	3.46	1.41		-4.5	-4.2	-6.2	0.00%	0.00%		0.00%
Distillates (petroleum), heavy thermal cracked	265-082-4	64741-81-7	64741817	-	-	5338	4.16	0.98	3	3.46	1.41		-4.5	-4.2	-6.2	0.00%	0.00%		0.00%
Naphtha (petroleum), full-range alkylate	265-066-7	64741-64-6	64741646	-	-	5339	4.13	0.46	3	3.13	0.46		-2.8	-3.1	-4.5	0.29%	0.10%		0.00%
Naphtha (petroleum), light hydrocracked	265-071-4	64741-69-1	64741691	-	-	5340	4.13	0.46	3	3.13	0.46		-4.5	-4.2	-6.2	0.00%	0.00%		0.00%
Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-deri	270-658-3	68475-70-7	68475707	-	-	5341	3.30	0.22	3	2.30	0.22		-4.5	-4.2	-6.2	0.00%	0.00%		0.00%
Naphtha (petroleum), heavy hydrocracked	265-079-8	64741-78-2	64741782	-	-	5342	4.13	0.46	3	3.13	0.46		-4.5	-4.2	-6.2	0.00%	0.00%		0.00%
Naphtha (petroleum), solvent-refined light	265-086-6	64741-84-0	64741840	-	-	5343	3.91	0.55	3	2.91	0.55		-4.5	-4.2	-6.2	0.00%	0.00%		0.00%
Residues (petroleum), topping plant, low-sulfur	271-763-7	68607-30-7	68607307	-	-	5344	4.16	0.98	3	3.46	1.41		-4.5	-4.2	-6.2	0.00%	0.00%		0.00%
Hydrocarbons, C4, steam-cracker distillate	295-405-4	92045-23-3	92045233	-	-	5345	4.17	0.21	3	3.17	0.21		-4.5	-4.2	-6.2	0.00%	0.00%		0.00%
Distillates (petroleum), solvent-refined heavy paraffinic	265-090-8	64741-88-4	64741884	-	-	5346	6.29	1.09	3	5.29	1.09		-4.5	-4.3	-6.2	0.00%	0.00%		0.00%
Aromatic hydrocarbons, C7-12, C8-rich	297-401-8	93571-75-6	93571756	-	-	5347	4.13	0.46	3	3.13	0.46		-4.5	-4.3	-6.2	0.00%	0.00%		0.00%
Naphtha (petroleum), light steam-cracked	265-187-5	64742-83-2	64742832	-	-	5348	3.30	0.22	3	2.30	0.22		-4.5	-4.3	-6.3	0.00%	0.00%		0.00%
Gas oils (petroleum), heavy atmospheric	272-184-2	68783-08-4	68783084	-	-	5349	4.16	0.98	3	3.46	1.41		-4.6	-4.3	-6.3	0.00%	0.00%		0.00%
Gases (petroleum), light steam-cracked, butadiene conc.	273-265-5	68955-28-2	68955282	-	-	5350	4.19	0.23	3	3.19	0.23		-4.6	-4.3	-6.3	0.00%	0.00%		0.00%
Distillates (petroleum), hydrotreated light	265-149-8	64742-47-8	64742478	-	-	5351	3.84	0.64	5	3.01	0.70		-4.6	-4.3	-6.3	0.00%	0.00%		0.00%
Naphtha (petroleum), light steam-cracked arom.	271-264-4	68527-23-1	68527231	-	-	5352	3.30	0.22	3	2.30	0.22		-4.6	-4.3	-6.3	0.00%	0.00%		0.00%
Clarified oils (petroleum), catalytic cracked	265-064-6	64741-62-4	64741624	-	-	5353	4.16	0.98	3	3.46	1.41		-4.6	-4.3	-6.3	0.00%	0.00%		0.00%
Distillates (petroleum), intermediate catalytic cracked	265-062-5	64741-60-2	64741602	-	-	5354	2.68	0.61	3	1.68	0.61		-4.6	-4.4	-6.3	0.00%	0.00%		0.00%
Gas oils (petroleum), thermal-cracked, hydrodesulfurized	295-411-7	92045-29-9	92045299	-	-	5355	2.68	0.61	3	1.68	0.61		-4.6	-4.4	-6.4	0.00%	0.00%		0.00%
Distillates (petroleum), hydrotreated heavy paraffinic	265-157-1	64742-54-7	64742547	-	-	5356	6.29	1.09	3	5.29	1.09		-4.6	-4.4	-6.4	0.00%	0.00%		0.00%
Gasoline, straight-run, topping-plant	271-727-0	68606-11-1	68606111	-	-	5357	4.13	0.46	3	3.13	0.46		-4.6	-4.4	-6.4	0.00%	0.00%		0.00%
Fuel oil, heavy, high-sulfur	295-396-7	92045-14-2	92045142	-	-	5358	4.16	0.98	3	3.46	1.41		-4.6	-4.4	-6.4	0.00%	0.00%		0.00%
Extracts (petroleum), heavy paraffinic distillate solvent	265-103-7	64742-04-7	64742047	-	-	5359	5.33	1.60	3	4.33	1.60		-4.7	-4.4	-6.4	0.00%	0.00%		0.00%
Hydrocarbons, ethylene-manuf.-by-product distn. residues	272-951-1	68921-67-5	68921675	-	-	5360	3.30	0.22	3	2.30	0.22		-4.7	-4.4	-6.4	0.00%	0.00%		0.00%
Hydrocarbons, C5-rich	270-695-5	68476-55-1	68476551	-	-	5361	4.12	0.43	3	3.12	0.43		-4.7	-4.4	-6.4	0.00%	0.00%		0.00%
Gasoline, C5-11, high-octane stabilized reformed	297-458-9	93572-29-3	93572293	-	-	5362	4.13	0.46	3	3.13	0.46		-4.7	-4.5	-6.4	0.00%	0.00%		0.00%
Distillates (petroleum), steam-cracked, C5-12 fraction	270-736-7	68477-53-2	68477532	-	-	5363	3.34	0.41	3	2.73	1.01		-4.7	-4.5	-6.4	0.00%	0.00%		0.00%
Gases (petroleum), crude distn. and catalytic cracking	273-563-5	68989-88-8	68989888	-	-	5364	4.41	0.39	3	3.41	0.39		-4.7	-4.5	-6.4	0.00%	0.00%		0.00%
Residues (petroleum), hydrodesulfurized atmospheric tower	265-181-2	64742-78-5	64742785	-	-	5365	4.16	0.98	3	3.46	1.41		-4.7	-4.5	-6.4	0.00%	0.00%		0.00%
Gas oils (petroleum), straight-run, high-boiling	272-818-8	68915-97-9	68915979	-	-	5366	4.26	0.61	3	3.59	0.60		-4.7	-4.5	-6.5	0.00%	0.00%		0.00%
Gas oils (petroleum), hydrodesulfurized light vacuum	265-190-1	64742-87-6	64742876	-	-	5367	4.28	0.58	3	3.55	0.52		-4.8	-4.5	-6.5	0.00%	0.00%		0.00%
Distillates (petroleum), light paraffinic	265-051-5	64741-50-0	64741500	-	-	5368	4.83	2.06	3	3.83	2.06		-4.8	-4.5	-6.5	0.00%	0.00%		0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Naphtha	232-443-2	8030-30-6	8030306	-	-	5369	3.78	0.49	9	2.78	0.70		-4.8	-4.5	-6.5	0.00%	0.00%	0.00%
Residues (petroleum), heavy coker gas oil and vacuum gas oil	270-796-4	68478-17-1	68478171	-	-	5370	4.22	0.96	3	3.61	1.29		-4.8	-4.5	-6.5	0.00%	0.00%	0.00%
Residues (petroleum), steam-cracked	265-193-8	64742-90-1	64742901	-	-	5371	3.62	0.53	3	2.99	0.69		-4.8	-4.6	-6.5	0.00%	0.00%	0.00%
Gases (petroleum), refinery blend	272-183-7	68783-07-3	68783073	-	-	5372	4.41	0.39	3	3.41	0.39		-4.8	-4.6	-6.5	0.00%	0.00%	0.00%
Distillates (petroleum), light thermal cracked, debutanized arom	273-266-0	68955-29-3	68955293	-	-	5373	3.30	0.22	3	2.30	0.22		-4.8	-4.6	-6.5	0.00%	0.00%	0.00%
Distillates (petroleum), light straight-run gasoline fractionation s	272-931-2	68921-08-4	68921084	-	-	5374	4.13	0.46	3	3.13	0.46		-4.8	-4.6	-6.5	0.00%	0.00%	0.00%
Solvent naphtha (petroleum), light aliph.	265-192-2	64742-89-8	64742898	-	-	5375	5.82	1.01	5	5.15	0.70		-4.8	-4.6	-6.5	0.00%	0.00%	0.00%
Residual oils (petroleum), solvent deasphalted	265-096-0	64741-95-3	64741953	-	-	5376	6.29	1.09	3	5.29	1.09		-4.8	-4.6	-6.6	0.00%	0.00%	0.00%
Kerosine (petroleum), straight-run wide-cut	295-418-5	92045-37-9	92045379	-	-	5377	4.13	0.46	3	3.13	0.46		-4.8	-4.6	-6.6	0.00%	0.00%	0.00%
Hydrocarbons, C3	271-735-4	68606-26-8	68606268	-	-	5378	4.41	0.39	3	3.41	0.39		-4.8	-4.6	-6.6	0.00%	0.00%	0.00%
Hydrocarbons, C5-7, C6-rich, ethylene manuf. by-products	294-557-9	91723-50-1	91723501	-	-	5379	3.30	0.22	3	2.30	0.22		-4.9	-4.6	-6.6	0.00%	0.00%	0.00%
Naphtha (petroleum), full-range coker	270-991-4	68513-02-0	68513020	-	-	5380	4.13	0.46	3	3.13	0.46		-4.9	-4.6	-6.6	0.00%	0.00%	0.00%
Distillates (petroleum), naphtha steam cracking-derived, hydrotr	295-311-3	91995-50-5	91995505	-	-	5381	3.30	0.22	3	2.30	0.22		-4.9	-4.6	-6.6	0.00%	0.00%	0.00%
Naphtha (petroleum), steam-cracked middle arom.	271-138-9	68516-20-1	68516201	-	-	5382	3.60	0.57	3	2.60	0.57		-4.9	-4.7	-6.6	0.00%	0.00%	0.00%
Natural gas condensates (petroleum)	265-047-3	64741-47-5	64741475	-	-	5383	3.98	0.54	3	2.98	0.54		-4.9	-4.7	-6.7	0.00%	0.00%	0.00%
Hydrocarbons, C"e5, C5-6-rich	270-690-8	68476-50-6	68476506	-	-	5384	4.13	0.46	3	3.13	0.46		-4.9	-4.7	-6.7	0.00%	0.00%	0.00%
Distillates (petroleum), heavy catalytic cracked	265-063-0	64741-61-3	64741613	-	-	5385	4.16	0.97	3	3.46	1.38		-4.9	-4.7	-6.7	0.00%	0.00%	0.00%
Gasoline, pyrolysis, hydrogenated	302-639-3	94114-03-1	94114031	-	-	5386	3.30	0.22	3	2.30	0.22		-4.9	-4.7	-6.7	0.00%	0.00%	0.00%
Slack wax (petroleum)	265-165-5	64742-61-6	64742616	-	-	5387	6.42	1.06	3	5.42	1.06		-4.9	-4.7	-6.7	0.00%	0.00%	0.00%
Fuel oil, residues-straight-run gas oils, high-sulfur	270-674-0	68476-32-4	68476324	-	-	5388	4.16	0.98	3	3.46	1.41		-5.0	-4.7	-6.7	0.00%	0.00%	0.00%
Distillates (petroleum), solvent-refined light paraffinic	265-091-3	64741-89-5	64741895	-	-	5389	6.29	1.09	3	5.29	1.09		-5.0	-4.7	-6.7	0.00%	0.00%	0.00%
Petroleum products, hydrofiner-powerformer reformates	271-058-4	68514-79-4	68514794	-	-	5390	4.13	0.46	3	3.13	0.46		-5.0	-4.7	-6.7	0.00%	0.00%	0.00%
Solvent naphtha (petroleum), light arom.	265-199-0	64742-95-6	64742956	-	-	5391	4.13	0.46	3	3.13	0.46		-5.0	-4.7	-6.7	0.00%	0.00%	0.00%
Gasoline, natural	232-349-1	8006-61-9	8006619	-	-	5392	4.13	0.46	3	3.13	0.46		-5.0	-4.7	-6.7	0.00%	0.00%	0.00%
Hydrocarbons, C3-11, catalytic cracker distillates	270-686-6	68476-46-0	68476460	-	-	5393	4.13	0.46	3	3.13	0.46		-5.0	-4.8	-6.7	0.00%	0.00%	0.00%
Residual oils (petroleum), solvent-refined	265-101-6	64742-01-4	64742014	-	-	5394	6.29	1.09	3	5.29	1.09		-5.0	-4.8	-6.7	0.00%	0.00%	0.00%
Residues (petroleum), steam-cracked light	271-013-9	68513-69-9	68513699	-	-	5395	3.55	0.49	3	2.92	0.77		-5.0	-4.8	-6.7	0.00%	0.00%	0.00%
Fuel gases, refinery	269-640-8	68308-27-0	68308270	-	-	5396	4.41	0.39	3	3.41	0.39		-5.0	-4.8	-6.8	0.00%	0.00%	0.00%
Distillates (petroleum), C6-rich	296-903-4	93165-19-6	93165196	-	-	5397	4.13	0.46	3	3.13	0.46		-5.0	-4.8	-6.8	0.00%	0.00%	0.00%
Naphtha (petroleum), light, sweetened	272-206-0	68783-66-4	68783664	-	-	5398	4.13	0.46	3	3.13	0.46		-5.0	-4.8	-6.8	0.00%	0.00%	0.00%
Residual oils (petroleum), solvent-dewaxed	265-166-0	64742-62-7	64742627	-	-	5399	6.29	1.09	3	5.29	1.09		-5.0	-4.8	-6.8	0.00%	0.00%	0.00%
Petroleum gases, liquefied	270-704-2	68476-85-7	68476857	-	-	5400	4.41	0.39	3	3.41	0.39		-5.0	-4.8	-6.8	0.00%	0.00%	0.00%
Naphtha (petroleum), light thermal cracked	265-075-6	64741-74-8	64741748	-	-	5401	4.13	0.46	3	3.13	0.46		-5.0	-4.8	-6.8	0.00%	0.00%	0.00%
Fuel oil, no. 4	270-673-5	68476-31-3	68476313	-	-	5402	4.26	0.59	3	3.56	0.49		-5.1	-4.8	-6.8	0.00%	0.00%	0.00%
Gases (petroleum), depropanizer dry, propene-rich	270-772-3	68477-90-7	68477907	-	-	5403	4.41	0.39	3	3.41	0.39		-5.1	-4.8	-6.8	0.00%	0.00%	0.00%
Hydrocarbons, C4-6, depentanizer lights, arom. hydrotreater	295-298-4	91995-38-9	91995389	-	-	5404	4.13	0.46	3	3.13	0.46		-5.1	-4.8	-6.8	0.00%	0.00%	0.00%
Residues (petroleum), vacuum distn. residue hydrogenation	309-713-4	100684-40-0	100684400	-	-	5405							-5.1	-4.8	-6.8	0.00%	0.00%	0.00%
Aromatic hydrocarbons, C8, catalytic reforming-derived	295-279-0	91995-18-5	91995185	-	-	5406	4.13	0.46	3	3.13	0.46		-5.1	-4.8	-6.8	0.00%	0.00%	0.00%
Condensates (petroleum), vacuum tower	265-049-4	64741-49-7	64741497	-	-	5407	4.28	0.58	3	3.55	0.51		-5.1	-4.8	-6.8	0.00%	0.00%	0.00%
Naphtha (petroleum), heavy thermal cracked	265-085-0	64741-83-9	64741839	-	-	5408	4.13	0.46	3	3.13	0.46		-5.1	-4.8	-6.8	0.00%	0.00%	0.00%
Distillates (petroleum), hydrotreated light paraffinic	265-158-7	64742-55-8	64742558	-	-	5409	6.29	1.09	3	5.29	1.09		-5.1	-4.8	-6.8	0.00%	0.00%	0.00%
Distillates (petroleum), hydrodesulfurized middle coker	309-865-1	101316-59-0	101316590	-	-	5410	2.68	0.62	3	1.68	0.62		-5.1	-4.9	-6.8	0.00%	0.00%	0.00%
Paraffin waxes and Hydrocarbon waxes	232-315-6	8002-74-2	8002742	-	-	5411	6.42	1.06	3	5.42	1.06		-5.1	-4.9	-6.8	0.00%	0.00%	0.00%
Distillates (petroleum), steam-cracked, C8-12 fraction	270-737-2	68477-54-3	68477543	-	-	5412	3.36	0.51	3	2.79	1.06		-5.1	-4.9	-6.8	0.00%	0.00%	0.00%
Residues (petroleum), hydrodesulfurized vacuum	265-188-0	64742-85-4	64742854	-	-	5413							-5.1	-4.9	-6.8	0.00%	0.00%	0.00%
Aromatic hydrocarbons, C7-8, ethylene-manuf.-by-product	292-699-6	90989-43-8	90989438	-	-	5414	3.30	0.22	3	2.30	0.22		-5.1	-4.9	-6.9	0.00%	0.00%	0.00%
Hydrocarbons, C4, 1,3-butadiene- and isobutene-free	306-004-1	95465-89-7	95465897	-	-	5415	4.15	0.21	3	3.15	0.21		-5.1	-4.9	-6.9	0.00%	0.00%	0.00%
Lubricating oils (petroleum), C20-50, hydrotreated neutral oil-ba	276-738-4	72623-87-1	72623871	-	-	5416	6.29	1.09	3	5.29	1.09		-5.1	-4.9	-6.9	0.00%	0.00%	0.00%
Solvent naphtha (petroleum), hydrocracked heavy arom.	309-881-9	101316-80-7	101316807	-	-	5417	4.01	0.65	3	3.01	0.67		-5.1	-4.9	-6.9	0.00%	0.00%	0.00%
Residues (petroleum), distn. residue hydrogenation	309-712-9	100684-39-7	100684397	-	-	5418							-5.2	-4.9	-6.9	0.00%	0.00%	0.00%
Solvent naphtha (petroleum), heavy arom.	265-198-5	64742-94-5	64742945	-	-	5419	3.80	0.63	3	3.01	0.73		-5.2	-4.9	-6.9	0.00%	0.00%	0.00%
Extracts (petroleum), catalytic reformed light naphtha solvent	295-331-2	91995-68-5	91995685	-	-	5420	4.13	0.46	3	3.13	0.46		-5.2	-4.9	-6.9	0.00%	0.00%	0.00%
Lubricating oils (petroleum), C24-50, solvent-extd., dewaxed, hy	309-877-7	101316-72-7	101316727	-	-	5421	6.29	1.09	3	5.29	1.09		-5.2	-4.9	-6.9	0.00%	0.00%	0.00%
Distillates (petroleum), hydrotreated middle, intermediate boilin	270-092-7	68410-96-8	68410968	-	-	5422	3.30	0.22	3	2.30	0.22		-5.2	-4.9	-6.9	0.00%	0.00%	0.00%
Distillates (petroleum), hydrotreated heavy naphthenic	265-155-0	64742-52-5	64742525	-	-	5423	6.29	1.07	3	5.29	1.07		-5.2	-4.9	-6.9	0.00%	0.00%	0.00%
Residues (petroleum), steam-cracked light, arom.	310-057-6	102110-55-4	102110554	-	-	5424	3.30	0.22	3	2.30	0.22		-5.2	-5.0	-6.9	0.00%	0.00%	0.00%
Naphtha (petroleum), light, C5-rich, sweetened	295-442-6	92045-60-8	92045608	-	-	5425	4.13	0.46	3	3.13	0.46		-5.2	-5.0	-7.0	0.00%	0.00%	0.00%
Gases (petroleum), catalytic cracked overheads	270-071-2	68409-99-4	68409994	-	-	5426	4.41	0.39	3	3.41	0.39		-5.2	-5.0	-7.0	0.00%	0.00%	0.00%
White mineral oil (petroleum)	232-455-8	8042-47-5	8042475	-	-	5427	5.61	0.42	3	4.61	0.42		-5.2	-5.0	-7.0	0.00%	0.00%	0.00%
Hydrocarbons, C3-4-rich, petroleum distillate	270-990-9	68512-91-4	68512914	-	-	5428	4.41	0.39	3	3.41	0.39		-5.3	-5.0	-7.0	0.00%	0.00%	0.00%
Slack wax (petroleum), clay-treated	292-660-3	90669-78-6	90669786	-	-	5429	6.42	1.06	3	5.42	1.06		-5.3	-5.0	-7.0	0.00%	0.00%	0.00%
Distillates (petroleum), hydrotreated light naphthenic	265-156-6	64742-53-6	64742536	-	-	5430	6.29	1.09	3	5.29	1.09		-5.3	-5.0	-7.0	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Naphtha (petroleum), heavy catalytic cracked, sweetened	295-431-6	92045-50-6	92045506	-	-	5431	4.13	0.46	3	3.13	0.46		-5.3	-5.0	-7.0	0.00%	0.00%	0.00%
Aromatic hydrocarbons, C8	292-694-9	90989-38-1	90989381	-	-	5432	3.62	0.26	3	2.62	0.26		-5.3	-5.0	-7.0	0.00%	0.00%	0.00%
Gases (petroleum), C3-5 olefinic-paraffinic alkylation feed	270-765-5	68477-83-8	68477838	-	-	5433	4.41	0.39	3	3.41	0.39		-5.3	-5.0	-7.0	0.00%	0.00%	0.00%
Hydrocarbons, C7-12, C>9-arom.-rich, reforming heavy fraction	297-465-7	93572-35-1	93572351	-	-	5434	4.13	0.46	3	3.13	0.46		-5.3	-5.1	-7.0	0.00%	0.00%	0.00%
Extracts (petroleum), residual oil solvent	265-110-5	64742-10-5	64742105	-	-	5435	5.68	0.75	3	4.68	0.75		-5.3	-5.1	-7.0	0.00%	0.00%	0.00%
Naphtha (petroleum), hydrodesulfurized full-range coker	309-879-8	101316-76-1	101316761	-	-	5436	4.13	0.46	3	3.13	0.46		-5.3	-5.1	-7.0	0.00%	0.00%	0.00%
Distillates (petroleum), solvent-dewaxed light paraffinic	265-159-2	64742-56-9	64742569	-	-	5437	6.29	1.09	3	5.29	1.09		-5.3	-5.1	-7.0	0.00%	0.00%	0.00%
Paraffin waxes (petroleum), hydrotreated	265-154-5	64742-51-4	64742514	-	-	5438	6.42	1.06	3	5.42	1.06		-5.3	-5.1	-7.1	0.00%	0.00%	0.00%
613-683-0	613-683-0	64741-72-6	64741726	-	-	5439	4.13	0.46	3	3.13	0.46		-5.3	-5.1	-7.1	0.00%	0.00%	0.00%
Naphtha (petroleum), catalytic reformed light, arom.-free fractic	285-510-3	85116-59-2	85116592	-	-	5440	4.13	0.46	3	3.13	0.46		-5.3	-5.1	-7.1	0.00%	0.00%	0.00%
Hydrocarbons, C6-rich, hydrotreated light naphtha distillates, so	309-871-4	101316-67-0	101316670	-	-	5441	4.13	0.46	3	3.13	0.46		-5.3	-5.1	-7.1	0.00%	0.00%	0.00%
Extracts (petroleum), light paraffinic distillate solvent	265-104-2	64742-05-8	64742058	-	-	5442	5.33	1.60	3	4.33	1.60		-5.3	-5.1	-7.1	0.00%	0.00%	0.00%
Gases (petroleum), C3-4	268-629-5	68131-75-9	68131759	-	-	5443	4.41	0.39	3	3.41	0.39		-5.3	-5.1	-7.1	0.00%	0.00%	0.00%
Hydrocarbons, C5-11, nonaroms.-rich, reforming light fraction	297-466-2	93572-36-2	93572362	-	-	5444	4.13	0.46	3	3.13	0.46		-5.4	-5.1	-7.1	0.00%	0.00%	0.00%
Distillates (petroleum), straight-run light	270-077-5	68410-05-9	68410059	-	-	5445	4.13	0.46	3	3.13	0.46		-5.4	-5.1	-7.1	0.00%	0.00%	0.00%
Hydrocarbons, C6-7, naphtha-cracking, solvent-refined	295-446-8	92045-64-2	92045642	-	-	5446	4.13	0.46	3	3.13	0.46		-5.4	-5.1	-7.1	0.00%	0.00%	0.00%
Distillates (petroleum), hydrotreated light catalytic cracked	272-930-7	68921-07-3	68921073	-	-	5447	2.68	0.62	3	1.68	0.62		-5.4	-5.1	-7.1	0.00%	0.00%	0.00%
Fuel gases, crude oil distillates	270-670-9	68476-29-9	68476299	-	-	5448	4.41	0.39	3	3.41	0.39		-5.4	-5.1	-7.1	0.00%	0.00%	0.00%
Naphtha (petroleum), isomerization, C6-fraction	295-440-5	92045-58-4	92045584	-	-	5449	4.13	0.46	3	3.13	0.46		-5.4	-5.1	-7.1	0.00%	0.00%	0.00%
Residues (petroleum), light vacuum	270-984-6	68512-62-9	68512629	-	-	5450	4.20	0.99	3	3.75	1.60		-5.4	-5.1	-7.1	0.00%	0.00%	0.00%
Naphtha (petroleum), light catalytic reformed, arom.-free	270-993-5	68513-03-1	68513031	-	-	5451	4.13	0.46	3	3.13	0.46		-5.4	-5.1	-7.1	0.00%	0.00%	0.00%
Naphtha (petroleum), steam-cracked, hydrotreated, C9-10-arom	292-637-8	90641-13-7	90641137	-	-	5452	3.30	0.22	3	2.30	0.22		-5.4	-5.1	-7.1	0.00%	0.00%	0.00%
Distillates (petroleum), sweetened middle	265-088-7	64741-86-2	64741862	-	-	5453	4.25	0.61	3	3.59	0.60		-5.4	-5.2	-7.1	0.00%	0.00%	0.00%
Distillates (petroleum), cracked steam-cracked petroleum distilla	270-727-8	68477-38-3	68477383	-	-	5454	3.64	0.54	3	2.99	0.69		-5.4	-5.2	-7.1	0.00%	0.00%	0.00%
Aromatic hydrocarbons, distn. residues, naphthalene-rich	308-487-4	98072-36-7	98072367	-	-	5455	3.64	0.54	3	2.99	0.69		-5.4	-5.2	-7.1	0.00%	0.00%	0.00%
Distillates (petroleum), catalytic reformed depentanizer	270-660-4	68475-79-6	68475796	-	-	5456	4.13	0.46	3	3.13	0.46		-5.4	-5.2	-7.2	0.00%	0.00%	0.00%
Naphtha (petroleum), light alkylate	265-068-8	64741-66-8	64741668	-	-	5457	4.13	0.46	3	3.13	0.46		-5.4	-5.2	-7.2	0.00%	0.00%	0.00%
Distillates (petroleum), cracked stripped steam-cracked petroleu	270-728-3	68477-39-4	68477394	-	-	5458	3.60	0.57	3	2.60	0.57		-5.4	-5.2	-7.2	0.00%	0.00%	0.00%
Residual oils (petroleum), hydrotreated	265-160-8	64742-57-0	64742570	-	-	5459	6.29	1.09	3	5.29	1.09		-5.4	-5.2	-7.2	0.00%	0.00%	0.00%
Residual oils (petroleum)	298-754-0	93821-66-0	93821660	-	-	5460	4.16	0.98	3	3.46	1.41		-5.4	-5.2	-7.2	0.00%	0.00%	0.00%
Distillates (petroleum), light steam-cracked naphtha	270-662-5	68475-80-9	68475809	-	-	5461	3.65	0.54	3	2.97	0.74		-5.4	-5.2	-7.2	0.00%	0.00%	0.00%
gases (petroleum), C3-4, isobutane-rich	270-724-1	68477-33-8	68477338	-	-	5462	4.41	0.39	3	3.41	0.39		-5.5	-5.2	-7.2	0.00%	0.00%	0.00%
Foots oil (petroleum)	265-171-8	64742-67-2	64742672	-	-	5463							-5.5	-5.2	-7.2	0.00%	0.00%	0.00%
Naphtha (petroleum), hydrotreated light steam-cracked	295-438-4	92045-57-3	92045573	-	-	5464	3.30	0.22	3	2.30	0.22		-5.5	-5.3	-7.2	0.00%	0.00%	0.00%
Hydrocarbons, C4-11, naphtha-cracking, arom.-free	295-445-2	92045-63-1	92045631	-	-	5465	4.13	0.46	3	3.13	0.46		-5.5	-5.3	-7.2	0.00%	0.00%	0.00%
Distillates (petroleum), light naphthenic	265-053-6	64741-52-2	64741522	-	-	5466	4.83	2.06	3	3.83	2.06		-5.5	-5.3	-7.2	0.00%	0.00%	0.00%
Paraffin oils (petroleum), catalytic dewaxed heavy	265-174-4	64742-70-7	64742707	-	-	5467	6.29	1.09	3	5.29	1.09		-5.5	-5.3	-7.3	0.00%	0.00%	0.00%
Distillates (petroleum), heavy naphthenic	265-054-1	64741-53-3	64741533	-	-	5468	4.83	2.06	3	3.83	2.06		-5.5	-5.3	-7.3	0.00%	0.00%	0.00%
Petrolatum	232-373-2	8009-03-8	8009038	-	-	5469	6.17	1.10	3	5.17	1.10		-5.6	-5.3	-7.3	0.00%	0.00%	0.00%
Slack wax (petroleum), hydrotreated	295-523-6	92062-09-4	92062094	-	-	5470	6.42	1.02	3	5.42	1.02		-5.6	-5.3	-7.3	0.00%	0.00%	0.00%
Alkanes, C12-26-branched and linear	292-454-3	90622-53-0	90622530	-	-	5471	4.25	0.61	3	3.59	0.60		-5.6	-5.3	-7.3	0.00%	0.00%	0.00%
Extracts (petroleum), solvent-refined heavy paraffinic distillate s	272-180-0	68783-04-0	68783040	-	-	5472	4.62	1.82	3	3.62	1.82		-5.6	-5.3	-7.3	0.00%	0.00%	0.00%
Hydrocarbons, C5-unsatd.	273-308-8	68956-55-8	68956558	-	-	5473	4.06	0.40	3	3.06	0.40		-5.6	-5.4	-7.3	0.00%	0.00%	0.00%
Hydrocarbons, C4-12, naphtha-cracking, hydrotreated	295-443-1	92045-61-9	92045619	-	-	5474	3.30	0.22	3	2.30	0.22		-5.6	-5.4	-7.3	0.00%	0.00%	0.00%
Gases (petroleum), C2-4, sweetened	272-205-5	68783-65-3	68783653	-	-	5475	4.41	0.39	3	3.41	0.39		-5.6	-5.4	-7.3	0.00%	0.00%	0.00%
Hydrocarbons, steam-cracking tar middle	289-222-9	86290-83-7	86290837	-	-	5476	3.64	0.54	3	2.99	0.69		-5.6	-5.4	-7.4	0.00%	0.00%	0.00%
Naphtha (petroleum), arom	271-635-0	68603-08-7	68603087	-	-	5477	4.13	0.46	3	3.13	0.46		-5.7	-5.4	-7.4	0.00%	0.00%	0.00%
Paraffin waxes and Hydrocarbon waxes, microcryst.	264-038-1	63231-60-7	63231607	-	-	5478	6.42	1.06	3	5.42	1.06		-5.7	-5.5	-7.5	0.00%	0.00%	0.00%
614-725-0	614-725-0	68783-11-9	68783119	-	-	5479	4.13	0.46	3	3.13	0.46		-5.7	-5.5	-7.5	0.00%	0.00%	0.00%
Gas oils (petroleum), steam-cracked	271-260-2	68527-18-4	68527184	-	-	5480	3.64	0.54	3	2.99	0.69		-5.7	-5.5	-7.5	0.00%	0.00%	0.00%
Naphtha (petroleum), catalytic dewaxed	265-170-2	64742-66-1	64742661	-	-	5481	4.13	0.46	3	3.13	0.46		-5.7	-5.5	-7.5	0.00%	0.00%	0.00%
Alkenes, C8-10-branched, C9-rich	307-301-9	97593-01-6	97593016	-	-	5482	2.97	0.81	3	3.48	1.86		-5.8	-5.5	-7.5	0.00%	0.00%	0.00%
Lubricating oils, used, vacuum distd.	295-422-7	92045-41-5	92045415	-	-	5483	3.84		2				-5.8	-5.5	-7.5	0.00%	0.00%	0.00%
Alkenes, C10-14-branched and linear, C12-rich	298-697-1	93821-12-6	93821126	-	-	5484	2.96	0.82	3	3.44	2.00		-5.8	-5.6	-7.5	0.00%	0.00%	0.00%
Hydrocarbons, C2-4, C3-rich	270-689-2	68476-49-3	68476493	-	-	5485	4.41	0.39	3	3.41	0.39		-5.8	-5.6	-7.5	0.00%	0.00%	0.00%
Distillates (petroleum), cracked, ethylene manuf. by-product, C9	305-586-4	94733-07-0	94733070	-	-	5486	3.36	0.51	3	2.79	1.06		-5.8	-5.6	-7.6	0.00%	0.00%	0.00%
Paraffin waxes (petroleum), clay-treated	265-145-6	64742-43-4	64742434	-	-	5487	6.42	1.02	3	5.42	1.02		-5.8	-5.6	-7.6	0.00%	0.00%	0.00%
Raffinates (petroleum), catalytic reformer ethylene glycol-water	270-088-5	68410-71-9	68410719	-	-	5488	4.13	0.46	3	3.13	0.46		-5.8	-5.6	-7.6	0.00%	0.00%	0.00%
Hydrocarbons, C4, n-butene conc.	306-005-7	95465-90-0	95465900	-	-	5489	4.15	0.21	3	3.15	0.21		-5.9	-5.6	-7.6	0.00%	0.00%	0.00%
Hydrocarbons, C3-6, C5-rich, steam-cracked naphtha	310-012-0	102110-14-5	102110145	-	-	5490	4.06	0.40	3	3.06	0.40		-5.9	-5.6	-7.6	0.00%	0.00%	0.00%
Gases (petroleum), catalytic-cracked gas oil depropanizer bottor	270-752-4	68477-71-4	68477714	-	-	5491	4.41	0.39	3	3.41	0.39		-5.9	-5.6	-7.6	0.00%	0.00%	0.00%
Petrolatum (petroleum), hydrotreated	295-459-9	92045-77-7	92045777	-	-	5492	6.17	1.10	3	5.17	1.10		-5.9	-5.6	-7.6	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Residues (petroleum), catalytic reformer fractionator	265-069-3	64741-67-9	64741679	-	-	5493	4.16	0.98	3	3.46	1.41		-5.9	-5.6	-7.6	0.00%	0.00%	0.00%
Lubricating oils (petroleum), C15-30, hydrotreated neutral oil-ba	276-737-9	72623-86-0	72623860	-	-	5494	6.29	1.09	3	5.29	1.09		-5.9	-5.7	-7.7	0.00%	0.00%	0.00%
Alkenes, C9-11, C10-rich	271-213-6	68526-56-7	68526567	-	-	5495	3.36	0.51	3	2.79	1.06		-5.9	-5.7	-7.7	0.00%	0.00%	0.00%
Gases (petroleum), refinery	272-338-9	68814-67-5	68814675	-	-	5496	4.41	0.39	3	3.41	0.39		-5.9	-5.7	-7.7	0.00%	0.00%	0.00%
Extracts (petroleum), deasphalted vacuum residue solvent	295-332-8	91995-70-9	91995709	-	-	5497	5.68	0.75	3	4.68	0.75		-5.9	-5.7	-7.7	0.00%	0.00%	0.00%
Lubricating oils (petroleum), C>25, solvent-extd., deasphalted, d	309-874-0	101316-69-2	101316692	-	-	5498	6.29	1.09	3	5.29	1.09		-6.0	-5.7	-7.7	0.00%	0.00%	0.00%
Gases (petroleum), deisobutanizer tower overheads	270-769-7	68477-87-2	68477872	-	-	5499	4.41	0.39	3	3.41	0.39		-6.0	-5.7	-7.7	0.00%	0.00%	0.00%
Dec-1-ene, trimers, hydrogenated	500-393-3	157707-86-3	157707863	-	-	5500	6.46	0.14	3	5.46	0.14		-6.0	-5.8	-7.8	0.00%	0.00%	0.00%
Hydrocarbons, C6-8, hydrogenated sorption-dearomatized, tolue	309-870-9	101316-66-9	101316669	-	-	5501	4.14	0.45	3	3.14	0.45		-6.1	-5.8	-7.8	0.00%	0.00%	0.00%
Extracts (petroleum), light naphtha solvent	265-100-0	64741-99-7	64741997	-	-	5502	3.30	0.22	3	2.30	0.22		-6.1	-5.8	-7.8	0.00%	0.00%	0.00%
Solvent naphtha (petroleum), heavy aliph.	265-200-4	64742-96-7	64742967	-	-	5503	4.01	0.65	3	3.01	0.67		-6.1	-5.8	-7.8	0.00%	0.00%	0.00%
Extracts (petroleum), heavy naphtha solvent	265-099-7	64741-98-6	64741986	-	-	5504	4.06	0.40	3	3.06	0.40		-6.1	-5.9	-7.8	0.00%	0.00%	0.00%
Distillates (petroleum), cracked stripped steam-cracked petroleu	270-729-9	68477-40-7	68477407	-	-	5505	3.36	0.52	3	2.79	1.10		-6.1	-5.9	-7.8	0.00%	0.00%	0.00%
Alkenes, C8-10, C9-rich	271-212-0	68526-55-6	68526556	-	-	5506	3.32	1.28	3	3.84	2.11		-6.1	-5.9	-7.8	0.00%	0.00%	0.00%
dodecene	246-922-9	25378-22-7	25378227	-	-	5507	3.38	1.23	3	2.38	1.23		-6.1	-5.9	-7.9	0.00%	0.00%	0.00%
Alkenes, C10-14	288-213-7	85681-75-0	85681750	-	-	5508	3.32	1.28	3	3.84	2.11		-6.1	-5.9	-7.9	0.00%	0.00%	0.00%
Distillates (petroleum), heat-soaked steam-cracked naphtha, C5-	295-302-4	91995-41-4	91995414	-	-	5509	4.07	0.39	3	3.07	0.39		-6.2	-5.9	-7.9	0.00%	0.00%	0.00%
Hydrocarbon waxes (petroleum), hydrotreated microcryst.	265-163-4	64742-60-5	64742605	-	-	5510	6.42	1.06	3	5.42	1.06		-6.2	-5.9	-7.9	0.00%	0.00%	0.00%
Hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fr	293-263-8	91053-01-9	91053019	-	-	5511	1.72	0.19	3	0.72	0.19		-6.3	-6.0	-8.0	0.00%	0.00%	0.00%
Hydrocarbon waxes (petroleum), clay-treated microcryst.	265-144-0	64742-42-3	64742423	-	-	5512	6.42	1.06	3	5.42	1.06		-6.3	-6.0	-8.0	0.00%	0.00%	0.00%
Distillates (petroleum), polymd. steam-cracked petroleum distill	270-735-1	68477-50-9	68477509	-	-	5513	3.67	0.58	3	2.92	0.99		-6.3	-6.0	-8.0	0.00%	0.00%	0.00%
Paraffin oils (petroleum), catalytic dewaxed light	265-176-5	64742-71-8	64742718	-	-	5514	6.29	1.09	3	5.29	1.09		-6.3	-6.0	-8.0	0.00%	0.00%	0.00%
Alkanes, C14-17	292-449-6	90622-47-2	90622472	-	-	5515	0.67		1				-6.3	-6.0	-8.0	0.00%	0.00%	0.00%
Hydrocarbons, C4, 1,3-butadiene-free, polymd., dibutylene fract	293-261-7	91052-99-2	91052992	-	-	5516	1.72	0.19	3	0.72	0.19		-6.3	-6.1	-8.0	0.00%	0.00%	0.00%
Gases (petroleum), butane splitter overheads	270-750-3	68477-69-0	68477690	-	-	5517	4.41	0.39	3	3.41	0.39		-6.3	-6.1	-8.0	0.00%	0.00%	0.00%
Distillates (petroleum), solvent-refined heavy naphthenic	265-097-6	64741-96-4	64741964	-	-	5518	6.29	1.09	3	5.29	1.09		-6.3	-6.1	-8.1	0.00%	0.00%	0.00%
Hydrocarbons, C4, butane conc., n-butene-contg.	306-006-2	95465-91-1	95465911	-	-	5519	4.15	0.21	3	3.15	0.21		-6.3	-6.1	-8.1	0.00%	0.00%	0.00%
Lubricating oils (petroleum), C18-40, solvent-dewaxed hydrocrac	305-594-8	94733-15-0	94733150	-	-	5520	6.29	1.09	3	5.29	1.09		-6.3	-6.1	-8.1	0.00%	0.00%	0.00%
Natural gas (petroleum), raw liq. mix	265-048-9	64741-48-6	64741486	-	-	5521	4.13	0.46	3	3.13	0.46		-6.3	-6.1	-8.1	0.00%	0.00%	0.00%
Hydrocarbons, C4-6, C5-rich	270-684-5	68476-43-7	68476437	-	-	5522	4.07	0.39	3	3.07	0.39		-6.3	-6.1	-8.1	0.00%	0.00%	0.00%
Distillates (petroleum), hydrodesulfurized thermal cracked midd	285-505-6	85116-53-6	85116536	-	-	5523	2.68	0.62	3	1.68	0.62		-6.4	-6.1	-8.1	0.00%	0.00%	0.00%
tridecene	246-919-2	25377-82-6	25377826	-	-	5524	5.37	2.30	3	4.37	2.30		-6.4	-6.1	-8.1	0.00%	0.00%	0.00%
Distillates (petroleum), catalytic reformed hydrotreated light, C8	285-509-8	85116-58-1	85116581	-	-	5525	4.13	0.46	3	3.13	0.46		-6.4	-6.1	-8.1	0.00%	0.00%	0.00%
Gases (petroleum), straight-run stabilizer off	272-883-2	68919-10-8	68919108	-	-	5526	4.41	0.39	3	3.41	0.39		-6.4	-6.1	-8.1	0.00%	0.00%	0.00%
Solvent naphtha (petroleum), medium aliph.	265-191-7	64742-88-7	64742887	-	-	5527	4.01	0.65	3	3.01	0.67		-6.4	-6.2	-8.1	0.00%	0.00%	0.00%
tetradecene	248-130-9	26952-13-6	26952136	-	-	5528	5.37	2.30	3	4.37	2.30		-6.4	-6.2	-8.2	0.00%	0.00%	0.00%
Gas oils (petroleum), hydrotreated light vacuum	295-407-5	92045-24-4	92045244	-	-	5529	4.28	0.58	3	3.55	0.52		-6.4	-6.2	-8.2	0.00%	0.00%	0.00%
Hydrocarbons, C9-14, ethylene-manuf.-by-product	271-035-9	68514-34-1	68514341	-	-	5530							-6.5	-6.2	-8.2	0.00%	0.00%	0.00%
Hydrocarbons, C9-16, hydrotreated, dearomatized	297-854-1	93763-35-0	93763350	-	-	5531	4.01	0.65	3	3.01	0.67		-6.5	-6.2	-8.2	0.00%	0.00%	0.00%
Residues (petroleum), alkylation splitter, C4-rich	271-010-2	68513-66-6	68513666	-	-	5532	4.41	0.39	3	3.41	0.39		-6.5	-6.2	-8.2	0.00%	0.00%	0.00%
Paraffin waxes and Hydrocarbon waxes, microcryst., hydrotreate	295-458-3	92045-76-6	92045766	-	-	5533	6.42	1.06	3	5.42	1.06		-6.5	-6.3	-8.3	0.00%	0.00%	0.00%
Naphtha (petroleum), light steam-cracked, debenzenized, C8-16	270-790-1	68478-10-4	68478104	-	-	5534	3.36	0.52	3	2.79	1.10		-6.5	-6.3	-8.3	0.00%	0.00%	0.00%
Petroleum gases, liquefied, sweetened, C4 fraction	295-463-0	92045-80-2	92045802	-	-	5535	4.41	0.39	3	3.41	0.39		-6.6	-6.3	-8.3	0.00%	0.00%	0.00%
Hydrocarbons, C17-30, hydrotreated distillates, distn. lights	308-132-3	97862-82-3	97862823	-	-	5536	6.29	1.09	3	5.29	1.09		-6.6	-6.3	-8.3	0.00%	0.00%	0.00%
Foots oil (petroleum), hydrotreated	295-394-6	92045-12-0	92045120	-	-	5537							-6.6	-6.3	-8.3	0.00%	0.00%	0.00%
Gas oils, paraffinic	300-227-8	93924-33-5	93924335	-	-	5538	4.25	0.61	3	3.59	0.60		-6.6	-6.3	-8.3	0.00%	0.00%	0.00%
Gases (petroleum), catalytic reformed naphtha stripper overhea	270-759-2	68477-77-0	68477770	-	-	5539	4.41	0.39	3	3.41	0.39		-6.6	-6.4	-8.3	0.00%	0.00%	0.00%
Benzenesulfonic acid, C16-24-alkyl derivs.	274-262-1	70024-67-8	70024678	-	-	5540	4.43	1.29	3	5.55	0.89		-6.6	-6.4	-8.4	0.00%	0.00%	0.00%
isoheptane	250-610-8	31394-54-4	31394544	-	-	5541	3.40	0.66	3	2.40	0.66		-6.7	-6.4	-8.4	0.00%	0.00%	0.00%
Sulfonic acids, petroleum, sodium salts	271-781-5	68608-26-4	68608264	-	-	5542	6.62	0.63	3	5.62	0.63		-6.7	-6.5	-8.5	0.00%	0.00%	0.00%
Naphtha (petroleum), hydrodesulfurized light, dearomatized	295-434-2	92045-53-9	92045539	-	-	5543	4.13	0.46	3	3.13	0.46		-6.7	-6.5	-8.5	0.00%	0.00%	0.00%
Distillates (petroleum), dewaxed light paraffinic, hydrotreated	295-301-9	91995-40-3	91995403	-	-	5544	6.29	1.09	3	5.29	1.09		-6.7	-6.5	-8.5	0.00%	0.00%	0.00%
Hydrocarbons, C4, 1,3-butadiene-free, polymd., dibutylene fract	297-626-1	93685-78-0	93685780	-	-	5545	1.72	0.19	3	0.72	0.19		-6.8	-6.5	-8.5	0.00%	0.00%	0.00%
Benzenesulfonic acid, mono-C16-24-alkyl derivs., calcium salts	274-263-7	70024-69-0	70024690	-	-	5546							-6.8	-6.6	-8.5	0.00%	0.00%	0.00%
Paraffins (petroleum), normal C>10	265-232-9	64771-71-7	64771717	-	-	5547				2.35			-6.8	-6.6	-8.5	0.00%	0.00%	0.00%
Benzenesulfonic acid, C14-44-branched and linear alkyl derivs., c	294-233-7	91696-74-1	91696741	-	-	5548	6.61	0.56	3	5.61	0.56		-6.8	-6.6	-8.5	0.00%	0.00%	0.00%
Hydrocarbons, C6-11, hydrotreated, dearomatized	297-852-0	93763-33-8	93763338	-	-	5549	4.13	0.46	3	3.13	0.46		-6.8	-6.6	-8.6	0.00%	0.00%	0.00%
Gases (petroleum), C1-5, wet	271-624-0	68602-83-5	68602835	-	-	5550	4.41	0.39	3	3.41	0.39		-6.8	-6.6	-8.6	0.00%	0.00%	0.00%
604-769-9	604-769-9	151006-63-2	151006632	-	-	5551	6.46	0.14	3	5.46	0.14		-6.9	-6.6	-8.6	0.00%	0.00%	0.00%
Naphthenic acids	215-662-8	1338-24-5	1338245	-	-	5552	3.96	0.35	6	2.96	0.35		-6.9	-6.6	-8.6	0.00%	0.00%	0.00%
618-143-8	618-143-8	883233-93-0	883233930	-	-	5553	6.46	0.14	3	5.46	0.14		-6.9	-6.7	-8.6	0.00%	0.00%	0.00%
Alkenes, C15-18	297-797-2	93762-80-2	93762802	-	-	5554	3.32	1.28	3	3.84	2.11		-7.0	-6.7	-8.7	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]		TP(Cwcoast) [-]
Distillates (petroleum), solvent-refined light naphthenic	265-098-1	64741-97-5	64741975	-	-	5555	6.29	1.09	3	5.29	1.09		-7.0	-6.7	-8.7	0.00%	0.00%		0.00%
618-141-7	618-141-7	883233-48-5	883233485	-	-	5556	6.46	0.14	3	5.46	0.14		-7.0	-6.8	-8.7	0.00%	0.00%		0.00%
Hydrocarbons, C4, 1,3-butadiene-free, polymd., tetraisobutylene	293-262-2	91053-00-8	91053008	-	-	5557	1.72	0.19	3	0.72	0.19		-7.0	-6.8	-8.7	0.00%	0.00%		0.00%
Petrolatum (petroleum), oxidized	265-206-7	64743-01-7	64743017	-	-	5558	6.17	1.03	3	5.17	1.03		-7.1	-6.8	-8.8	0.00%	0.00%		0.00%
Sulfonic acids, petroleum, calcium salts	263-093-9	61789-86-4	61789864	-	-	5559							-7.1	-6.8	-8.8	0.00%	0.00%		0.00%
Lubricating oils (petroleum), base oils, paraffinic	297-474-6	93572-43-1	93572431	-	-	5560	6.50	0.82	3	5.50	0.82		-7.1	-6.8	-8.8	0.00%	0.00%		0.00%
Benzenesulfonic acid, C10-16-alkyl derivs., calcium salts	271-529-4	68584-23-6	68584236	-	-	5561	6.62	0.63	3	5.62	0.63		-7.1	-6.8	-8.8	0.00%	0.00%		0.00%
Distillates (petroleum), chemically neutralized light	265-132-5	64742-31-0	64742310	-	-	5562	4.01	0.65	3	3.01	0.67		-7.1	-6.8	-8.8	0.00%	0.00%		0.00%
Benzene, ethylenated, residues	273-494-0	68987-42-8	68987428	-	-	5563	3.64	0.54	3	2.99	0.69		-7.1	-6.8	-8.8	0.00%	0.00%		0.00%
Lubricating oils (petroleum), C20-50, hydrotreated neutral oil-ba	276-736-3	72623-85-9	72623859	-	-	5564	6.29	1.07	3	5.29	1.07		-7.1	-6.9	-8.8	0.00%	0.00%		0.00%
Ligroine	232-453-7	8032-32-4	8032324	-	-	5565	4.13	0.46	3	3.13	0.46		-7.1	-6.9	-8.8	0.00%	0.00%		0.00%
Paraffin oils	232-384-2	8012-95-1	8012951	-	-	5566	4.31	2.07	6	3.87	0.70		-7.2	-6.9	-8.9	0.00%	0.00%		0.00%
618-142-2	618-142-2	883233-91-8	883233918	-	-	5567	6.46	0.14	3	5.46	0.14		-7.2	-6.9	-8.9	0.00%	0.00%		0.00%
Residues, steam cracked, thermally treated	308-733-0	98219-64-8	98219648	-	-	5568	3.64	0.54	3	2.99	0.69		-7.2	-6.9	-8.9	0.00%	0.00%		0.00%
tetrapropylenebenzene	246-772-4	25265-78-5	25265785	-	-	5569							-7.2	-6.9	-8.9	0.00%	0.00%		0.00%
Distillates (petroleum), solvent-refined hydrotreated heavy, hyd	305-588-5	94733-08-1	94733081	-	-	5570	6.29	1.09	3	5.29	1.09		-7.2	-7.0	-9.0	0.00%	0.00%		0.00%
Benzenesulfonic acid, C10-60-alkyl derivs., calcium salts	290-636-7	90194-27-7	90194277	-	-	5571	6.62	0.63	3	5.62	0.63		-7.2	-7.0	-9.0	0.00%	0.00%		0.00%
Benzenesulfonic acid, C10-16-alkyl derivs.	271-528-9	68584-22-5	68584225	-	-	5572	6.62	0.63	3	5.62	0.63		-7.2	-7.0	-9.0	0.00%	0.00%		0.00%
octene	246-920-8	25377-83-7	25377837	-	-	5573	3.32	1.28	3	3.84	2.11		-7.4	-7.1	-9.1	0.00%	0.00%		0.00%
Hydrocarbon waxes (petroleum), oxidized	265-205-1	64743-00-6	64743006	-	-	5574	5.50		3	4.50			-7.4	-7.1	-9.1	0.00%	0.00%		0.00%
Residual oils (petroleum), catalytic dewaxed	294-843-3	91770-57-9	91770579	-	-	5575	6.29	1.09	3	5.29	1.09		-7.4	-7.1	-9.1	0.00%	0.00%		0.00%
Paraffins (petroleum), normal C5-20	265-233-4	64771-72-8	64771728	-	-	5576							-7.4	-7.1	-9.1	0.00%	0.00%		0.00%
Foots oil (petroleum), clay-treated	300-226-2	93924-32-4	93924324	-	-	5577							-7.4	-7.2	-9.1	0.00%	0.00%		0.00%
Sulfonic acids, petroleum, magnesium salts	263-094-4	61789-87-5	61789875	-	-	5578	6.66	0.60	3	5.66	0.60		-7.4	-7.2	-9.2	0.00%	0.00%		0.00%
Benzenesulfonic acid, C10-16-alkyl derivs., magnesium salts	271-533-6	68584-26-9	68584269	-	-	5579	6.66	0.60	3	5.66	0.60		-7.4	-7.2	-9.2	0.00%	0.00%		0.00%
Residual oils (petroleum), hydrotreated solvent dewaxed	292-656-1	90669-74-2	90669742	-	-	5580	6.29	1.09	3	5.29	1.09		-7.4	-7.2	-9.2	0.00%	0.00%		0.00%
Sulfonic acids, petroleum	263-092-3	61789-85-3	61789853	-	-	5581	6.62	0.63	3	5.62	0.63		-7.5	-7.2	-9.2	0.00%	0.00%		0.00%
Distillates (petroleum), clay-treated heavy naphthenic	265-146-1	64742-44-5	64742445	-	-	5582	6.29	1.09	3	5.29	1.09		-7.5	-7.2	-9.2	0.00%	0.00%		0.00%
Naphtha (petroleum), heavy alkylate	265-067-2	64741-65-7	64741657	-	-	5583							-7.6	-7.3	-9.3	0.00%	0.00%		0.00%
Lubricating oils, used, distd.	295-421-1	92045-40-4	92045404	-	-	5584							-7.6	-7.3	-9.3	0.00%	0.00%		0.00%
2-Methylpropene, trimers	500-001-0	7756-94-7	7756947	-	-	5585	1.72	0.19	3	0.72	0.19		-7.6	-7.4	-9.4	0.00%	0.00%		0.00%
Petrolatum (petroleum), clay-treated	309-706-6	100684-33-1	100684331	-	-	5586	6.17	1.10	3	5.17	1.10		-7.7	-7.5	-9.4	0.00%	0.00%		0.00%
Petrolatum (petroleum), oxidized, Bu ester	292-642-5	90669-48-0	90669480	-	-	5587	5.41	0.13	3	4.41	0.13		-8.0	-7.8	-9.8	0.00%	0.00%		0.00%
Hydrocarbon waxes (petroleum), oxidized, Me esters, calcium sa	271-638-7	68603-11-2	68603112	-	-	5588	5.67	0.61	3	4.67	0.61		-8.1	-7.9	-9.8	0.00%	0.00%		0.00%
Sulfonic acids, petroleum, barium salts	263-140-3	61790-48-5	61790485	-	-	5589	6.66	0.60	3	5.66	0.60		-8.1	-7.9	-9.9	0.00%	0.00%		0.00%
Benzenesulfonic acid, di-C10-18-alkyl derivs., barium salts	298-635-3	93820-55-4	93820554	-	-	5590	6.66	0.60	3	5.66	0.60		-8.1	-7.9	-9.9	0.00%	0.00%		0.00%
800-484-0	800-484-0	154518-38-4	154518384	-	-	5591	4.48	0.38	3	3.25	0.54		-8.2	-7.9	-9.9	0.00%	0.00%		0.00%
Hydrocarbons, C4, 1,3-butadiene-free, polymd., pentaisobutylen	297-627-7	93685-79-1	93685791	-	-	5592	7.67		1				-8.2	-8.0	-9.9	0.00%	0.00%		0.00%
Alkenes, C14-15	297-796-7	93762-79-9	93762799	-	-	5593							-8.2	-8.0	-9.9	0.00%	0.00%		0.00%
Extracts (petroleum), heavy paraffinic distillates, solvent-deasph	272-342-0	68814-89-1	68814891	-	-	5594				5.22			-8.6	-8.4	-10.4	0.00%	0.00%		0.00%
Benzene, C9-13-alkyl derivs., distn. residues, sulfonated, calcium	307-593-8	97675-24-6	97675246	-	-	5595	6.08	0.83	3	5.08	0.83		-8.7	-8.4	-10.4	0.00%	0.00%		0.00%
Ethylbenzene, manuf. of, distn. residues, distn. lights.	700-371-5	178535-25-6	178535256	-	-	5596	3.38		2				-9.0	-8.8	-10.8	0.00%	0.00%		0.00%
Benzene, mono-C10-14-alkyl derivs., fractionation bottoms, inte	285-597-8	85117-47-1	85117471	-	-	5597	6.08	0.83	3	5.08	0.83		-9.7	-9.5	-11.4	0.00%	0.00%		0.00%
Pharmaceuticals																			
count							*167*	*158*	*167*	*54*	*50*	*10*	*392*	*392*	*392*	*392*	*392*	*1.3%*	*392*
sum																*0.004%*	*0.007%*	*98.9%*	*0.0001%*
standard deviation							*1.14*	*0.52*		*1.226*	*0.60*		*1.7*	*1.7*	*1.9*				
2.5-p													*-11.9*	*-12.1*	*-14.1*	*6.6E-33*	*8.2E-34*		*3.8E-45*
50-p							*3.82*	*0.72*	*3*	*3.00*	*0.97*	*15*	*-8.1*	*-8.1*	*-9.7*	*2.9E-16*	*2.3E-16*		*1.1E-22*
97.5-p													*-5.5*	*-5.4*	*-6.6*	*1.5E-08*	*2.7E-08*		*2.6E-11*
Paracetamol		103-90-2	103902	165	Reach_616	5599	5.22	0.81	9	2.11	1.11		-4.0	-3.8	-4.7	0.00%	0.01%	0.006%	0.00%
Metformin Hydrochloride (Metformin)		657-24-9	657249	79	PharmaBeta_488	5600	5.37	0.58	4	4.37	0.58		-4.4	-4.4	-5.9	0.00%	0.00%	0.007%	0.00%
Phenobarbital		50-06-6	50066	4945	PharmaBeta_244	5601	5.84	0.28	3	4.84	0.28		-4.8	-4.8	-6.6	0.00%	0.00%	0.007%	0.00%
Naproxen		22204-53-1	22204531	539	PharmaBeta_529	5602	4.33	1.12	10	3.33	1.12		-5.0	-4.8	-5.8	0.00%	0.00%	0.007%	0.00%
Ibuprofen		15687-27-1	15687271	493	Reach_2393	5603	4.31	0.73	20	2.38	1.84	16	-5.1	-4.9	-6.0	0.00%	0.00%	0.007%	0.00%
Gabapentin		604-75-1	604751	72	PharmaBeta_286	5604	3.55	0.80	3				-5.0	-4.9	-6.0	0.00%	0.00%		0.00%
Carbamazepine		298-46-4	298464	45	PharmaBeta_372	5605	4.59	0.41	19	2.38	1.25	19	-5.4	-5.2	-6.3	0.00%	0.00%		0.00%
Tramadol Hydrochloride		27203-92-5	27203925	41	PharmaBeta_757	5606	3.62	0.65	3				-5.5	-5.3	-6.5	0.00%	0.00%		0.00%
Amoxicillin		26787-78-0	26787780	574	Reach_2594	5607							-5.4	-5.4	-7.0	0.00%	0.00%		0.00%
RANITIDINE		66357-35-5	66357355	789	Reach_2879	5608	5.00	0.88	4	4.00	0.88		-5.5	-5.4	-6.6	0.00%	0.00%		0.00%
Diclofenac		15307-86-5	15307865	31	Reach_2382	5609	4.31	0.63	17	1.93	1.50	14	-5.6	-5.5	-6.4	0.00%	0.00%		0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Furosemide		54-31-9	54319	62	PharmaBeta_284	5610	2.45	1.94	4	1.45	1.94		-5.7	-5.5	-6.5	0.00%	0.00%	0.00%
Omeprazole		73590-58-6	73590586	832	PharmaBeta_573	5611	4.94		1				-5.7	-5.6	-6.7	0.00%	0.00%	0.00%
Phenoxymethylpenicillin (Penicillin V)		87-08-01	870801	-	-	5612							-5.8	-5.6	-7.1	0.00%	0.00%	0.00%
Valproic Acid		202409-33-4	202409334	2256	PharmaBeta_231	5613							-5.7	-5.6	-6.7	0.00%	0.00%	0.00%
Cholestyramine		11041-12-6	11041126	-	-	5614							-5.8	-5.6	-7.1	0.00%	0.00%	0.00%
Lamotrigine		84057-84-1	84057841	102	PharmaBeta_428	5615	4.76	0.17	3	3.76	0.17		-5.8	-5.7	-6.5	0.00%	0.00%	0.00%
Sulfamethoxazol		723-46-6	723466	86	PharmaBeta_703	5616	3.98	1.36	15	2.36	1.29	24	-5.8	-5.7	-7.2	0.00%	0.00%	0.00%
Mebeverine Hydrochloride		2753-45-9	2753459	6362	PharmaUBA	5617							-5.9	-5.7	-7.2	0.00%	0.00%	0.00%
Theophylline		65807-02-5	65807025	730	Reach_47	5618							-5.8	-5.7	-6.6	0.00%	0.00%	0.00%
STRONTIUM		165800-03-3	165800033	504	PharmaBeta_452	5619	4.13	1.06	3	4.58			-5.9	-5.8	-7.0	0.00%	0.00%	0.00%
flucloxacillin		5250-39-5	5250395	3062	PharmaBeta_260	5620	3.57	0.72	3				-5.9	-5.8	-7.6	0.00%	0.00%	0.00%
PROPRANOLOL HYDROCHLORIDE		7722-84-1	7722841	6452	PharmaBeta_779	5621	4.44	0.72	9	4.54	1.26		-6.0	-5.9	-7.3	0.00%	0.00%	0.00%
Diltiazem Hydrochloride （Diltiazem）		42399-41-7	42399417	637	PharmaBeta_173	5622	4.24		2				-6.0	-5.9	-7.4	0.00%	0.00%	0.00%
Oxytetracycline		79-57-2	79572	923	PharmaBeta_583	5623	4.34	1.13	15	3.99	1.21	7	-5.9	-5.9	-7.4	0.00%	0.00%	0.00%
Thiamine Hydrochloride		59467-70-8	59467708	736	PharmaBeta_502	5624							-6.0	-5.9	-7.1	0.00%	0.00%	0.00%
Allopurinol		315-30-0	315300	2628	PharmaBeta_24	5625							-5.8	-5.9	-7.7	0.00%	0.00%	0.00%
Bezafibrate		41859-67-0	41859670	53	PharmaBeta_89	5626	4.64	0.69	9	1.69	2.91		-6.0	-5.9	-7.3	0.00%	0.00%	0.00%
Simvastatin		79902-63-9	79902639	927	PharmaBeta_689	5627	4.36		1				-5.8	-5.9	-7.5	0.00%	0.00%	0.00%
Clopidogrel		113665-84-2	113665842	8	PharmaBeta_405	5628	2.98	0.41	3				-6.1	-5.9	-7.3	0.00%	0.00%	0.00%
Erythromycin		114-07-8	114078	336	Reach_933	5629	4.19	1.35	17	2.15	2.09	11	-6.1	-6.0	-7.6	0.00%	0.00%	0.00%
Atenolol		298-46-4	298464	44	PharmaBeta_58	5630	4.59	0.41	19	2.38	1.25	19	-5.9	-6.0	-7.7	0.00%	0.00%	0.00%
Cefalexin		15686-71-2	15686712	492	PharmaBeta_117	5631	3.00		1				-6.1	-6.0	-7.2	0.00%	0.00%	0.00%
VERAPAMIL HYDROCHLORIDE		119478-56-7	119478567	5622	PharmaBeta_483	5632							-6.2	-6.0	-7.5	0.00%	0.00%	0.00%
Amitriptyline		54024-22-5	54024225	662	Reach_8	5633							-6.1	-6.0	-7.1	0.00%	0.00%	0.00%
Sertraline		79617-96-2	79617962	924	PharmaBeta_684	5634	2.58	0.70	10	1.67	0.87		-6.2	-6.0	-7.1	0.00%	0.00%	0.00%
MORPHINE		57-27-2	57272	721	PharmaBeta_518	5635	3.49	0.45	3	3.00			-6.2	-6.0	-7.0	0.00%	0.00%	0.00%
Hydroxychloroquine Sulphate		16679-58-6	16679586	6397	PharmaBeta_159	5636							-6.2	-6.1	-7.5	0.00%	0.00%	0.00%
Trimethoprim		738-70-5	738705	89	PharmaBeta_765	5637	4.70	1.29	33	4.11	1.06		-6.1	-6.1	-7.6	0.00%	0.00%	0.00%
Clarithromycin		81103-11-9	81103119	99	PharmaBeta_391	5638	3.45	1.80	8	2.45	1.29		-6.3	-6.1	-7.8	0.00%	0.00%	0.00%
Celecoxib		169590-42-5	169590425	508	PharmaBeta_124	5639	3.33	1.13	3	2.47			-6.3	-6.1	-7.0	0.00%	0.00%	0.00%
Hydrochlorothiazide		58-93-5	58935	69	PharmaBeta_318	5640	5.22	1.56	3				-6.2	-6.1	-7.2	0.00%	0.00%	0.00%
Aspirin		50-78-2	50782	666	Reach_9	5641							-6.3	-6.2	-8.2	0.00%	0.00%	0.00%
Ursodeoxycholic Acid		214766-78-6	214766786	6424	PharmaBeta_156	5642							-6.4	-6.2	-7.7	0.00%	0.00%	0.00%
Irbesartan		138402-11-6	138402116	444	PharmaBeta_343	5643	5.34	0.33	3	3.80	0.52		-6.2	-6.2	-7.6	0.00%	0.00%	0.00%
Sitagliptin		486460-32-6	486460326	2974	Reach_4660	5644	3.82	1.81	3				-6.3	-6.2	-7.6	0.00%	0.00%	0.00%
Ketoprofen		22071-15-4	22071154	38	PharmaBeta_384	5645	3.93	0.48	3				-6.4	-6.2	-7.1	0.00%	0.00%	0.00%
Etodolac		120287-85-6	120287856	6418	PharmaBeta_126	5646							-6.4	-6.2	-7.7	0.00%	0.00%	0.00%
Cimetidine		51481-61-9	51481619	1129	PharmaUBA	5647	5.59	0.39	4	4.59	0.39		-6.3	-6.3	-7.6	0.00%	0.00%	0.00%
Mefenamic Acid		61-68-7	61687	1150	PharmaUBA	5648	3.82	0.17	5	2.82	0.17		-6.1	-6.3	-7.4	0.00%	0.00%	0.00%
Valsartan		137862-53-4	137862534	442	PharmaBeta_775	5649							-6.4	-6.3	-7.8	0.00%	0.00%	0.00%
Sucralfate		39474-58-3	39474583	6377	PharmaUBA	5650							-6.5	-6.3	-7.8	0.00%	0.00%	0.00%
Flutamide		13311-84-7	13311847	427	PharmaBeta_270	5651	3.85	0.80	4	2.85	0.80		-6.5	-6.3	-7.2	0.00%	0.00%	0.00%
Lansoprazole		103577-45-3	103577453	1372	PharmaBeta_430	5652							-6.4	-6.3	-8.1	0.00%	0.00%	0.00%
Mirtazapine		61337-67-5	61337675	-	-	5653							-6.5	-6.4	-7.8	0.00%	0.00%	0.00%
Amlodipine		88150-42-9	88150429	982	PharmaBeta_42	5654	3.16	0.81	3	1.92	1.24		-6.5	-6.4	-8.0	0.00%	0.00%	0.00%
Nifedipine		21829-25-4	21829254	1102	PharmaBeta_549	5655	3.66	1.34	3				-6.5	-6.4	-7.8	0.00%	0.00%	0.00%
Lidocaine		137-58-6	137586	26	PharmaBeta_451	5656	3.55	0.50	3				-6.5	-6.4	-7.5	0.00%	0.00%	0.00%
MYCOPHENOLATE		139264-17-8	139264178	1918	PharmaBeta_800	5657	2.91	0.60	3				-6.3	-6.4	-8.1	0.00%	0.00%	0.00%
Codeine Phosphate (Codeine)		76-57-3	76573	3719	PharmaBeta_416	5658	3.56	0.54	3				-6.2	-6.4	-8.4	0.00%	0.00%	0.00%
Sulfasalazine		599-79-1	599791	3300	PharmaBeta_704	5659	3.48	0.58	3				-6.4	-6.4	-8.5	0.00%	0.00%	0.00%
Miconazole		22916-47-8	22916478	5364	PharmaUBA	5660	1.74	0.05	3				-6.4	-6.5	-7.5	0.00%	0.00%	0.00%
Nitrofurantoin		67-20-9	67209	791	PharmaBeta_557	5661	4.51	1.29	9	3.51	1.29		-6.4	-6.5	-8.0	0.00%	0.00%	0.00%
Docusate Sodium		198904-31-3	198904313	2244	PharmaBeta_57	5662	3.13	0.89	3				-6.6	-6.5	-8.2	0.00%	0.00%	0.00%
Ketoconazole		65277-42-1	65277421	78	PharmaBeta_383	5663	3.23	0.35	3	2.06			-6.6	-6.5	-7.6	0.00%	0.00%	0.00%
Gliclazide		29110-47-2	29110472	5323	PharmaUBA	5664	3.64	0.87	3				-6.4	-6.5	-8.6	0.00%	0.00%	0.00%
Betamethasone		378-44-9	378449	619	Reach_1261	5665							-6.7	-6.6	-8.0	0.00%	0.00%	0.00%
Quinine		130-95-0	130950	5427	PharmaUBA	5666	3.50	0.60	3				-6.6	-6.6	-8.6	0.00%	0.00%	0.00%
Temazepam		147127-20-6	147127206	5457	PharmaUBA	5667							-6.7	-6.6	-7.7	0.00%	0.00%	0.00%
Calcium Acetate		1492-18-8	1492188	6274	PharmaBeta_363	5668							-6.8	-6.6	-8.1	0.00%	0.00%	0.00%
Diazepam		439-14-5	439145	640	PharmaBeta_166	5669	3.74	0.32	3	2.74	0.32		-6.8	-6.7	-7.8	0.00%	0.00%	0.00%
Amantadine Hydrochloride		66592-87-8	66592878	5982	PharmaBeta_116	5670							-6.8	-6.7	-8.1	0.00%	0.00%	0.00%
Prednisolone		50-24-8	50248	656	Reach_6	5671	4.30	1.42	3	3.30	1.42		-6.8	-6.7	-8.2	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [·]	Z(Cwfresh) [·]	Z(Cwcoast) [·]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
FLUOXETINE		54910-89-3	54910893	692	PharmaBeta_268	5672	3.78	1.39	11	1.53	0.90	8	-6.8	-6.7	-8.3	0.00%	0.00%	0.00%
Atorvastatin		134523-00-5	134523005	431	PharmaBeta_60	5673	2.60	1.31	3	1.61	2.74		-6.6	-6.7	-8.2	0.00%	0.00%	0.00%
Oxazepam		604-75-1	604751	73	PharmaBeta_579	5674	3.55	0.80	3				-6.8	-6.7	-7.8	0.00%	0.00%	0.00%
Dipyridamole		58-32-2	58322	3243	PharmaBeta_178	5675	4.96	0.83	3				-6.7	-6.7	-8.8	0.00%	0.00%	0.00%
Cefadroxil		66592-87-8	66592878	5982	PharmaBeta_116	5676							-6.9	-6.7	-8.2	0.00%	0.00%	0.00%
Fluconazole		86386-73-4	86386734	970	PharmaBeta_261	5677	4.79	0.37	3	3.79	0.37		-6.9	-6.8	-7.6	0.00%	0.00%	0.00%
Hydrocortisone		50-23-7	50237	655	Reach_5	5678	4.88	0.30	3				-6.9	-6.8	-8.4	0.00%	0.00%	0.00%
Tetracycline		60-54-8	60548	754	PharmaBeta_731	5679	3.63	0.91	7	2.42	1.46		-6.8	-6.8	-8.4	0.00%	0.00%	0.00%
Tranexamic Acid		274901-16-5	274901165	2510	PharmaBeta_786	5680	4.32	1.39	3				-6.6	-6.9	-8.9	0.00%	0.00%	0.00%
Aciclovir		51-52-5	51525	5108	PharmaBeta_637	5681	4.36	0.59	3	3.36	0.75		-6.8	-6.9	-8.9	0.00%	0.00%	0.00%
Felodipine		72519-76-3	72519763	-	-	5682							-7.1	-6.9	-8.3	0.00%	0.00%	0.00%
Mesalazine (Systemic)		89-57-6	89576	3980	Reach_345	5683	4.69	0.54	3	3.69	0.54		-6.5	-6.9	-8.9	0.00%	0.00%	0.00%
Fenofibrate		49562-28-9	49562289	649	Reach_2761	5684	4.42	1.04	12	3.42	1.04		-6.9	-6.9	-8.2	0.00%	0.00%	0.00%
Timolol		26839-75-8	26839758	2488	PharmaBeta_740	5685	4.28	0.91	3				-6.8	-6.9	-8.9	0.00%	0.00%	0.00%
Isoniazid		54910-89-3	54910893	691	PharmaBeta_346	5686	3.78	1.39	11	1.53	0.90	8	-7.0	-6.9	-7.8	0.00%	0.00%	0.00%
Losartan Potassium		5633-20-5	5633205	3190	PharmaBeta_585	5687	3.56	0.43	3				-6.9	-6.9	-8.9	0.00%	0.00%	0.00%
Methocarbamol		61-32-5	61325	5360	PharmaUBA	5688	4.21	0.95	3				-6.6	-6.9	-9.0	0.00%	0.00%	0.00%
Dihydrocodeine		125-28-0	125280	5283	PharmaUBA	5689	3.89	0.69	3				-6.8	-6.9	-9.0	0.00%	0.00%	0.00%
Venlafaxine		58-46-8	58468	5154	PharmaBeta_730	5690	3.28	0.48	3				-7.1	-7.0	-9.0	0.00%	0.00%	0.00%
Primidone		125-33-7	125337	5420	PharmaUBA	5691	4.19	1.15	3				-6.9	-7.0	-8.7	0.00%	0.00%	0.00%
Balsalazide Sodium		38304-91-5	38304915	2820	PharmaBeta_508	5692	4.47	1.40	3				-6.6	-7.0	-9.0	0.00%	0.00%	0.00%
Disulfiram		97-77-8	97778	1060	Reach_487	5693	2.35	0.78	6	1.26	0.65		-7.1	-7.0	-8.1	0.00%	0.00%	0.00%
Nitrazepam		146-22-5	146225	474	PharmaBeta_556	5694	6.00		1				-7.2	-7.0	-8.2	0.00%	0.00%	0.00%
Levodopa		59-92-7	59927	745	PharmaBeta_444	5695	4.20	1.04	6	3.20	1.04		-6.7	-7.0	-9.0	0.00%	0.00%	0.00%
Acetylcysteine		616-91-1	616911	3348	PharmaBeta_5	5696	4.84	0.19	3				-6.7	-7.0	-9.1	0.00%	0.00%	0.00%
Fexofenadine Hydrochloride		93-14-1	93141	4061	PharmaBeta_312	5697	5.65	0.76	3				-6.7	-7.0	-9.1	0.00%	0.00%	0.00%
Azithromycin		83905-01-5	83905015	957	Reach_4465	5698							-7.1	-7.0	-8.7	0.00%	0.00%	0.00%
Quetiapine		143322-58-1	143322581	1963	PharmaBeta_199	5699	2.58	0.30	3				-6.9	-7.0	-9.1	0.00%	0.00%	0.00%
Lymecycline		158966-92-8	158966928	2066	PharmaBeta_517	5700	0.73	2.53	3				-7.0	-7.0	-7.8	0.00%	0.00%	0.00%
Carbocisteine		638-23-3	638233	5239	PharmaUBA	5701	5.70	1.15	3				-6.4	-7.0	-9.1	0.00%	0.00%	0.00%
Cinnarizine		298-57-5	298575	-	-	5702							-7.2	-7.1	-8.5	0.00%	0.00%	0.00%
Nicotinic Acid		59-67-6	59676	739	Reach_52	5703	5.29	0.61	4	4.29	0.61		-7.0	-7.1	-9.0	0.00%	0.00%	0.00%
Oxycodone		76-42-6	76426	3711	PharmaBeta_581	5704	3.88	0.74	3				-7.0	-7.1	-8.8	0.00%	0.00%	0.00%
Etoricoxib		202409-33-4	202409334	2256	PharmaBeta_231	5705	2.79	0.23	3				-7.2	-7.1	-8.2	0.00%	0.00%	0.00%
Disopyramide		3737-09-5	3737095	115	PharmaBeta_179	5706	5.00		2				-7.3	-7.1	-8.3	0.00%	0.00%	0.00%
Finasteride		98319-26-7	98319267	1070	PharmaBeta_253	5707	4.31		2				-7.3	-7.1	-8.5	0.00%	0.00%	0.00%
Captopril		62571-86-2	62571862	1103	PharmaUBA	5708							-7.3	-7.1	-8.6	0.00%	0.00%	0.00%
Gemfibrozil		25812-30-0	25812300	570	PharmaBeta_299	5709	4.54	1.04	42	1.94	1.91		-7.1	-7.1	-8.2	0.00%	0.00%	0.00%
Zopiclone		43200-80-2	43200802	2908	PharmaBeta_803	5710	3.01	0.40	3				-7.0	-7.1	-8.9	0.00%	0.00%	0.00%
Crotamiton		3546-03-0	3546030	5266	PharmaUBA	5711							-7.4	-7.2	-8.9	0.00%	0.00%	0.00%
Phenytoin		57-41-0	57410	3229	PharmaBeta_250	5712	3.71	0.90	3				-7.1	-7.2	-9.2	0.00%	0.00%	0.00%
Indometacin		21829-25-4	21829254	1101	PharmaBeta_338	5713	3.66	1.34	3				-7.2	-7.2	-8.7	0.00%	0.00%	0.00%
Urea		57-13-6	57136	719	Reach_39	5714	6.56	0.97	12	6.20	0.70	20	-7.4	-7.2	-9.1	0.00%	0.00%	0.00%
Levetiracetam		27262-47-1	27262471	5007	PharmaBeta_442	5715	2.93	0.26	3				-6.9	-7.2	-9.3	0.00%	0.00%	0.00%
Carvedilol		72956-09-3	72956093	826	PharmaBeta_379	5716	3.00	1.04	9	1.70	1.04		-7.3	-7.2	-8.7	0.00%	0.00%	0.00%
Acamprosate Calcium		55-98-1	55981	708	PharmaBeta_110	5717	4.00		1				-6.9	-7.2	-9.3	0.00%	0.00%	0.00%
Meloxicam		71125-39-8	71125398	-	-	5718							-7.4	-7.2	-8.7	0.00%	0.00%	0.00%
Hydrogen Peroxide		7722-84-1	7722841	6452	PharmaBeta_779	5719	4.44	0.72	9	4.54	1.26		-7.4	-7.2	-8.7	0.00%	0.00%	0.00%
Aminophylline		183321-74-6	183321746	2183	PharmaBeta_216	5720	3.17	0.64	3				-7.2	-7.2	-9.3	0.00%	0.00%	0.00%
Aminophylline		183321-74-6	183321746	2183	PharmaBeta_216	5721	3.17	0.64	3				-7.2	-7.2	-9.3	0.00%	0.00%	0.00%
Ergocalciferol (Vitamin D2)		78755-81-4	78755814	4957	PharmaBeta_262	5722	4.17	0.83	3				-7.0	-7.2	-9.3	0.00%	0.00%	0.00%
Carbidopa		745-65-3	745653	3640	PharmaBeta_27	5723	3.16	0.45	3				-7.2	-7.2	-9.3	0.00%	0.00%	0.00%
Lisinopril		83915-83-7	83915837	3852	PharmaBeta_454	5724	4.56	0.94	3				-6.8	-7.3	-9.3	0.00%	0.00%	0.00%
Isosorbide		53123-88-9	53123889	3089	PharmaBeta_690	5725	2.49	0.65	3				-7.4	-7.3	-9.2	0.00%	0.00%	0.00%
Ramipril		87333-19-5	87333195	3928	PharmaBeta_646	5726	4.02	0.57	3				-7.3	-7.3	-9.3	0.00%	0.00%	0.00%
Sodium Citrate		1716-12-7	1716127	6294	PharmaBeta_533	5727							-7.5	-7.3	-8.8	0.00%	0.00%	0.00%
CLINDAMYCIN		18323-44-9	18323449	2181	PharmaBeta_394	5728	4.59	0.77	3				-7.2	-7.3	-9.4	0.00%	0.00%	0.00%
Norfloxacin		70458-96-7	70458967	812	PharmaBeta_562	5729							-7.4	-7.3	-8.4	0.00%	0.00%	0.00%
Chlordiazepoxide		58-25-3	58253	1127	PharmaUBA	5730							-7.4	-7.3	-8.5	0.00%	0.00%	0.00%
Nicotine		66085-59-4	66085594	5067	PharmaBeta_551	5731	3.30	1.50	3				-7.5	-7.4	-9.1	0.00%	0.00%	0.00%
Ofloxacin		82419-36-1	82419361	945	PharmaBeta_568	5732							-7.5	-7.4	-8.3	0.00%	0.00%	0.00%
Pregabalin		148553-50-8	148553508	2003	PharmaBeta_626	5733	4.57	0.91	3				-6.8	-7.4	-9.5	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION					EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Testosterone		58-22-0	58220	67	Reach_46	5734	3.10	1.66	3	2.10	1.66		-7.5	-7.4	-9.2	0.00%	0.00%	0.00%
Sildenafil		1397-89-3	1397893	1923	PharmaBeta_688	5735	4.13	0.93	3				-7.5	-7.4	-9.2	0.00%	0.00%	0.00%
Chloral Hydrate		302-17-0	302170	1126	PharmaUBA	5736							-7.7	-7.5	-8.7	0.00%	0.00%	0.00%
PRAVASTATIN		53-03-2	53032	5101	PharmaBeta_623	5737	4.98	0.84	3				-7.4	-7.5	-9.5	0.00%	0.00%	0.00%
Sulfadiazine		68-35-9	68359	1165	PharmaUBA	5738							-7.6	-7.5	-8.3	0.00%	0.00%	0.00%
Lacosamide		585-86-4	585864	4999	PharmaBeta_425	5739	9.09	3.38	3				-7.4	-7.5	-9.3	0.00%	0.00%	0.00%
Clozapine		5786-251-0	57862510	-	-	5740							-7.7	-7.5	-9.0	0.00%	0.00%	0.00%
Rifampicin		133040-01-4	133040014	1863	PharmaBeta_656	5741	3.14	0.47	3				-7.7	-7.5	-9.3	0.00%	0.00%	0.00%
Oxcarbazepine		28721-07-5	28721075	2541	PharmaBeta_584	5742	3.84	0.87	3				-7.3	-7.5	-9.6	0.00%	0.00%	0.00%
TERBINAFINE		91161-71-6	91161716	4012	Reach_4498	5743	1.78		2				-7.6	-7.5	-9.4	0.00%	0.00%	0.00%
Demeclocycline Hydrochloride		64-73-3	64733	5969	Reach_74	5744							-7.7	-7.5	-9.0	0.00%	0.00%	0.00%
Sulpiride		15676-16-1	15676161	5454	PharmaUBA	5745	4.67	0.85	3				-7.2	-7.5	-9.6	0.00%	0.00%	0.00%
Levofloxacin		100986-85-4	100986854	139	PharmaBeta_445	5746							-7.6	-7.5	-8.4	0.00%	0.00%	0.00%
ZUCLOPENTHIXOL		53772-83-1	53772831	3109	PharmaBeta_804	5747							-7.7	-7.6	-8.5	0.00%	0.00%	0.00%
Abacavir		136470-78-5	136470785	1899	PharmaBeta_2	5748	3.69	1.49	3				-7.5	-7.6	-9.6	0.00%	0.00%	0.00%
FLUVASTATIN		93957-54-1	93957541	4094	PharmaBeta_272	5749	2.57	0.54	3				-7.6	-7.6	-9.0	0.00%	0.00%	0.00%
Ampicillin		69-53-4	69534	808	Reach_94	5750							-7.7	-7.6	-8.8	0.00%	0.00%	0.00%
Methotrexate		59-05-2	59052	732	PharmaBeta_492	5751							-7.6	-7.6	-8.8	0.00%	0.00%	0.00%
Clotrimazole		23593-75-1	23593751	553	PharmaBeta_413	5752	1.58	0.69	8	0.58	0.69		-7.3	-7.6	-8.9	0.00%	0.00%	0.00%
Progesterone		57-83-0	57830	65	Reach_43	5753	3.78	0.08	3				-7.8	-7.6	-9.4	0.00%	0.00%	0.00%
Nortriptyline		67018-85-3	67018853	5392	PharmaUBA	5754	2.04	1.54	3				-7.8	-7.6	-9.4	0.00%	0.00%	0.00%
Triamterene		396-01-1	396011	-	-	5755							-7.8	-7.6	-9.1	0.00%	0.00%	0.00%
Indapamide		26807-65-8	26807658	5332	PharmaUBA	5756							-7.8	-7.7	-9.1	0.00%	0.00%	0.00%
Fluorouracil		51333-22-3	51333223	669	PharmaBeta_104	5757							-7.8	-7.7	-8.9	0.00%	0.00%	0.00%
Methylprednisolone		83-43-2	83432	3846	PharmaBeta_498	5758	4.96	0.49	3				-7.6	-7.7	-9.7	0.00%	0.00%	0.00%
Citalopram Hydrobromide (Citalopram)		72559-06-9	72559069	3606	PharmaBeta_655	5759							-7.3	-7.7	-9.0	0.00%	0.00%	0.00%
Domperidone		57808-66-9	57808669	5289	PharmaUBA	5760	3.32	0.32	3				-7.6	-7.7	-9.7	0.00%	0.00%	0.00%
GLYCEROL		56-81-5	56815	716	Reach_30	5761	6.94	0.39	6	5.94	0.39		-7.6	-7.7	-9.8	0.00%	0.00%	0.00%
Medroxyprogesterone Acetate		4928-02-3	4928023	5213	PharmaUBA	5762	3.98	0.67	3				-7.8	-7.7	-9.5	0.00%	0.00%	0.00%
DULOXETINE		116539-59-4	116539594	1652	PharmaBeta_193	5763	2.69	0.37	3				-7.9	-7.7	-9.7	0.00%	0.00%	0.00%
Nadolol		1404-04-2	1404042	1154	PharmaUBA	5764							-7.9	-7.7	-8.9	0.00%	0.00%	0.00%
Mebendazole		31431-39-7	31431397	599	PharmaBeta_470	5765							-7.9	-7.7	-8.7	0.00%	0.00%	0.00%
Budesonide		51333-22-3	51333223	669	PharmaBeta_104	5766							-7.9	-7.7	-8.9	0.00%	0.00%	0.00%
Famotidine		76824-35-6	76824356	1100	PharmaBeta_239	5767							-7.9	-7.8	-8.9	0.00%	0.00%	0.00%
Sodium Benzoate		532-32-1	532321	1218	Reach_1329	5768							-8.0	-7.8	-9.2	0.00%	0.00%	0.00%
Imipramine		50-49-7	50497	5330	PharmaUBA	5769	2.75	0.47	3				-7.9	-7.8	-9.5	0.00%	0.00%	0.00%
Hyoscine Hydrobromide		114-49-8	114498	5612	Reach_934	5770							-8.0	-7.8	-9.3	0.00%	0.00%	0.00%
Nevirapine		129618-40-2	129618402	1829	PharmaBeta_548	5771	3.79	0.92	3				-7.9	-7.8	-9.6	0.00%	0.00%	0.00%
DOXAZOSIN		74191-85-8	74191858	3633	PharmaBeta_187	5772	3.54	0.99	3				-7.6	-7.8	-9.9	0.00%	0.00%	0.00%
MEMANTINE		19982-08-2	19982082	2246	PharmaBeta_480	5773	3.66	0.69	3				-8.1	-7.8	-9.5	0.00%	0.00%	0.00%
Pantoprazole		102625-70-7	102625707	1349	PharmaBeta_592	5774							-7.7	-7.8	-9.9	0.00%	0.00%	0.00%
TAMOXIFEN		10540-29-1	10540291	174	Reach_2294	5775	1.76	0.13	3				-7.7	-7.9	-9.1	0.00%	0.00%	0.00%
Orlistat		96-88-8	96888	4154	PharmaBeta_576	5776	3.59	0.50	3				-7.5	-7.9	-8.9	0.00%	0.00%	0.00%
Flurbiprofen		23155-02-4	23155024	5319	PharmaUBA	5777	6.30	0.48	3				-8.1	-7.9	-9.7	0.00%	0.00%	0.00%
Pentoxifylline		6493-05-6	6493056	5409	PharmaUBA	5778	3.96	1.25	3				-7.7	-7.9	-9.9	0.00%	0.00%	0.00%
Diethylamine Salicylate （Diethylamine）		142217-69-4	142217694	4922	PharmaBeta_205	5779	5.25	1.49	3				-7.4	-7.9	-9.9	0.00%	0.00%	0.00%
Risperidone		106266-06-2	106266062	188	PharmaBeta_660	5780							-8.1	-7.9	-8.9	0.00%	0.00%	0.00%
Itraconazole		84625-61-6	84625616	3872	PharmaBeta_351	5781	2.64	1.15	3				-7.7	-7.9	-9.3	0.00%	0.00%	0.00%
Calcium Gluconate		471-34-1	471341	6276	PharmaBeta_365	5782							-8.1	-8.0	-9.4	0.00%	0.00%	0.00%
Fluocinolone Acetonide		67-73-2	67732	1142	PharmaUBA	5783							-8.1	-8.0	-9.5	0.00%	0.00%	0.00%
Modafinil		68693-11-8	68693118	3525	PharmaBeta_514	5784							-7.9	-8.0	-10.0	0.00%	0.00%	0.00%
Griseofulvin		23210-56-2	23210562	1144	PharmaUBA	5785							-8.1	-8.0	-9.7	0.00%	0.00%	0.00%
Ezetimibe		163222-33-1	163222331	2088	PharmaBeta_237	5786	2.91	0.26	3				-8.0	-8.0	-10.1	0.00%	0.00%	0.00%
Azelaic Acid		123-99-9	123999	1782	Reach_1064	5787							-8.1	-8.1	-10.1	0.00%	0.00%	0.00%
Escitalopram		128196-01-0	128196010	1817	PharmaBeta_219	5788	2.91	0.36	3				-8.2	-8.1	-10.1	0.00%	0.00%	0.00%
Ropinirole		287714-41-4	287714414	5125	PharmaBeta_667	5789							-8.3	-8.1	-9.9	0.00%	0.00%	0.00%
Nilotinib		641571-10-0	641571100	3427	Reach_4930	5790	2.29	0.17	3				-8.0	-8.1	-10.1	0.00%	0.00%	0.00%
Aliskiren		154323-57-6	154323576	4834	PharmaBeta_23	5791	3.35	0.13	3				-8.1	-8.1	-10.2	0.00%	0.00%	0.00%
Linezolid		165800-03-3	165800033	504	PharmaBeta_452	5792							-8.3	-8.1	-9.3	0.00%	0.00%	0.00%
Telmisartan		144701-48-4	144701484	1981	PharmaBeta_719	5793	2.59	1.76	3				-7.9	-8.1	-9.1	0.00%	0.00%	0.00%
Olanzapine		132539-06-1	132539061	1859	PharmaBeta_570	5794	3.54	0.54	3				-8.1	-8.1	-10.2	0.00%	0.00%	0.00%
Dexamethasone		50-02-2	50022	652	PharmaBeta_161	5795							-8.3	-8.1	-9.5	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Cyclophosphamide		50-18-0	50180	1131	PharmaUBA	5796							-8.3	-8.1	-9.0	0.00%	0.00%	0.00%
Menthol		89-78-1	89781	994	Reach_351	5797							-8.4	-8.2	-9.8	0.00%	0.00%	0.00%
Desloratadine		100643-71-8	100643718	1308	PharmaBeta_158	5798							-8.3	-8.2	-9.9	0.00%	0.00%	0.00%
VANCOMYCIN		37332-99-3	37332993	6458	PharmaUBA	5799							-8.3	-8.2	-9.6	0.00%	0.00%	0.00%
Triclosan		3380-34-5	3380345	48	Reach_1954	5800							-8.3	-8.2	-9.1	0.00%	0.00%	0.00%
Sulfapyridine		144-83-2	144832	29	Reach_1196	5801							-8.4	-8.2	-9.0	0.00%	0.00%	0.00%
Chloramphenicol		56-75-7	56757	64	PharmaBeta_407	5802							-8.2	-8.2	-9.6	0.00%	0.00%	0.00%
Loratadine		79794-75-5	79794755	3783	PharmaBeta_460	5803	3.15	0.25	3				-8.2	-8.2	-10.1	0.00%	0.00%	0.00%
Glibenclamide		10238-21-8	10238218	152	PharmaBeta_301	5804							-8.2	-8.2	-9.7	0.00%	0.00%	0.00%
Chloroquine Phosphate		50-63-5	50635	6280	PharmaBeta_410	5805							-8.4	-8.2	-9.7	0.00%	0.00%	0.00%
Montelukast		158966-92-8	158966928	2066	PharmaBeta_517	5806	0.73	2.53	3				-8.3	-8.2	-9.0	0.00%	0.00%	0.00%
Estradiol		50-28-2	50282	55	Reach_7	5807							-8.3	-8.2	-9.6	0.00%	0.00%	0.00%
Oxybutynin		5633-20-5	5633205	3190	PharmaBeta_585	5808	3.56	0.43	3				-8.2	-8.3	-10.3	0.00%	0.00%	0.00%
Clonazepam		1622-61-3	1622613	500	PharmaBeta_403	5809							-8.4	-8.3	-9.5	0.00%	0.00%	0.00%
Levonorgestrel		79794-75-5	79794755	3782	PharmaBeta_448	5810	3.15	0.25	3				-8.3	-8.3	-10.3	0.00%	0.00%	0.00%
Tinidazole		193-91-8	193918	-	-	5811							-8.5	-8.3	-9.7	0.00%	0.00%	0.00%
Digoxin		2098-66-0	2098660	529	PharmaBeta_169	5812							-8.3	-8.3	-9.8	0.00%	0.00%	0.00%
Tolfenamic Acid		13710-19-5	13710195	1177	PharmaUBA	5813							-8.1	-8.3	-9.5	0.00%	0.00%	0.00%
CEFUROXIME		55268-75-2	55268752	3165	PharmaBeta_123	5814	5.45	1.44	3				-8.0	-8.3	-10.4	0.00%	0.00%	0.00%
Chlorothiazide		58-94-6	58946	5255	PharmaUBA	5815							-8.2	-8.3	-10.1	0.00%	0.00%	0.00%
Nystatin		1400-61-9	1400619	1925	PharmaBeta_567	5816	1.67	0.30	3				-8.0	-8.3	-9.8	0.00%	0.00%	0.00%
Nicotinamide		98-92-0	98920	1079	Reach_524	5817							-8.3	-8.3	-10.0	0.00%	0.00%	0.00%
Lorazepam		846-49-1	846491	103	PharmaBeta_461	5818							-8.4	-8.3	-9.4	0.00%	0.00%	0.00%
Promethazine		60-87-7	60877	5422	PharmaUBA	5819	2.76	0.33	3				-8.5	-8.3	-10.3	0.00%	0.00%	0.00%
Albendazole		54965-21-8	54965218	1121	PharmaUBA	5820							-8.5	-8.3	-9.3	0.00%	0.00%	0.00%
Rufinamide		89365-50-4	89365504	5128	PharmaBeta_673	5821	3.30	0.08	3				-8.4	-8.4	-10.5	0.00%	0.00%	0.00%
Salbutamol		18559-94-9	18559949	2198	Reach_2465	5822	3.40	0.96	3				-8.1	-8.4	-10.4	0.00%	0.00%	0.00%
Norethisterone		68-22-4	68224	800	Reach_92	5823							-8.5	-8.4	-10.1	0.00%	0.00%	0.00%
Piracetam		7491-74-9	7491749	3651	PharmaBeta_612	5824	4.34	1.54	3				-7.8	-8.4	-10.5	0.00%	0.00%	0.00%
Salicylic Acid		69-72-7	69727	84	Reach_95	5825	5.24	1.02	7	4.15	0.57		-8.4	-8.4	-10.5	0.00%	0.00%	0.00%
Glipizide		29094-61-9	29094619	4968	PharmaBeta_303	5826	3.60	1.82	3				-8.4	-8.4	-10.5	0.00%	0.00%	0.00%
Propylthiouracil		51-52-5	51525	5108	PharmaBeta_637	5827	4.36	0.59	3	3.36	0.75		-8.4	-8.4	-10.5	0.00%	0.00%	0.00%
Meprobamate		57-53-4	57534	5358	PharmaUBA	5828	4.98	1.10	3				-8.6	-8.5	-10.5	0.00%	0.00%	0.00%
Lofepramine		23047-25-8	23047258	5348	PharmaUBA	5829	1.79	0.16	3				-8.1	-8.5	-9.9	0.00%	0.00%	0.00%
Sevelamer		19767-45-4	19767454	5019	PharmaBeta_485	5830	4.02	0.79	3				-7.8	-8.5	-10.3	0.00%	0.00%	0.00%
Imiquimod		26807-65-8	26807658	5331	PharmaUBA	5831							-8.6	-8.5	-10.3	0.00%	0.00%	0.00%
Cefradine		38821-53-3	38821533	5252	PharmaUBA	5832							-8.0	-8.5	-10.6	0.00%	0.00%	0.00%
Ketamine		6740-88-1	6740881	3490	PharmaBeta_381	5833							-8.7	-8.5	-10.3	0.00%	0.00%	0.00%
Meropenem		119478-56-7	119478567	5622	PharmaBeta_483	5834							-8.7	-8.5	-10.0	0.00%	0.00%	0.00%
Ephedrine Hydrochloride		50-98-6	50986	5902	Reach_11	5835							-8.7	-8.5	-10.0	0.00%	0.00%	0.00%
Dapsone		80-08-0	80080	3787	Reach_256	5836	4.00	0.81	3	3.00	0.81		-8.4	-8.5	-10.6	0.00%	0.00%	0.00%
Perindopril		82834-16-0	82834160	5090	PharmaBeta_604	5837	4.55	0.87	3				-8.3	-8.5	-10.5	0.00%	0.00%	0.00%
Sulfinpyrazone		15676-16-1	15676161	5453	PharmaUBA	5838							-8.4	-8.5	-10.6	0.00%	0.00%	0.00%
Ribavirin		36791-04-5	36791045	2778	PharmaBeta_654	5839	6.67	2.33	3				-7.9	-8.5	-10.6	0.00%	0.00%	0.00%
Eprosartan		133040-01-4	133040014	1864	PharmaBeta_210	5840	3.14	0.47	3				-8.4	-8.5	-10.2	0.00%	0.00%	0.00%
Vardenafil		224785-90-4	224785904	2334	Reach_4232	5841							-8.6	-8.5	-10.3	0.00%	0.00%	0.00%
Exemestane		104227-87-4	104227874	5306	PharmaUBA	5842							-8.7	-8.5	-10.6	0.00%	0.00%	0.00%
Doxepin		469-21-6	469216	5291	PharmaUBA	5843	3.45	0.61	3				-8.8	-8.5	-10.6	0.00%	0.00%	0.00%
Haloperidol		52-86-8	52868	3079	PharmaBeta_313	5844							-8.7	-8.5	-9.7	0.00%	0.00%	0.00%
Nateglinide		105816-04-4	105816044	5060	PharmaBeta_531	5845	3.13	0.59	3				-8.5	-8.6	-10.6	0.00%	0.00%	0.00%
Tadalafil		209860-87-7	209860877	5139	PharmaBeta_710	5846							-8.4	-8.6	-10.6	0.00%	0.00%	0.00%
Acipimox		578-95-0	578950	5216	PharmaUBA	5847							-8.3	-8.6	-10.6	0.00%	0.00%	0.00%
Fusidic Acid		6990-06-3	6990063	5322	PharmaUBA	5848	3.30	0.25	3				-8.3	-8.6	-10.2	0.00%	0.00%	0.00%
LEVOMEPROMAZINE		60-99-1	60991	3322	PharmaBeta_447	5849	2.80	0.46	3				-8.6	-8.6	-10.6	0.00%	0.00%	0.00%
Teicoplanin		108736-35-2	108736352	6461	PharmaUBA	5850							-8.8	-8.6	-10.1	0.00%	0.00%	0.00%
Tiaprofenic Acid		33005-95-7	33005957	5463	PharmaUBA	5851							-8.8	-8.6	-10.7	0.00%	0.00%	0.00%
Dexibuprofen		24584-09-6	24584096	4891	PharmaBeta_163	5852							-8.9	-8.6	-10.6	0.00%	0.00%	0.00%
Lormetazepam		1977-10-2	1977102	5350	PharmaUBA	5853							-8.7	-8.6	-9.6	0.00%	0.00%	0.00%
Piroxicam		33817-20-8	33817208	5417	PharmaUBA	5854	4.65	0.87	3				-8.4	-8.7	-10.7	0.00%	0.00%	0.00%
VILDAGLIPTIN		274901-16-5	274901165	2510	PharmaBeta_786	5855							-8.4	-8.7	-10.7	0.00%	0.00%	0.00%
Mupirocin		126544-47-6	126544476	1806	PharmaBeta_522	5856							-8.6	-8.7	-10.7	0.00%	0.00%	0.00%
Midazolam		59467-70-8	59467708	736	PharmaBeta_502	5857							-8.8	-8.7	-9.8	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Isosorbide Dinitrate		87-33-2	87332	3926	Reach_308	5858							-8.6	-8.7	-10.8	0.00%	0.00%	0.00%
Dasatinib		201530-41-8	201530418	4888	PharmaBeta_151	5859							-8.7	-8.7	-10.5	0.00%	0.00%	0.00%
Ivabradine		78649-41-9	78649419	4986	PharmaBeta_352	5860							-8.7	-8.7	-10.8	0.00%	0.00%	0.00%
Megestrol Acetate		3562-63-8	3562638	5355	PharmaUBA	5861							-8.7	-8.8	-10.8	0.00%	0.00%	0.00%
Colchicine		64-86-8	64868	782	Reach_75	5862							-8.9	-8.8	-10.4	0.00%	0.00%	0.00%
Deferasirox		30652-11-0	30652110	4889	PharmaBeta_153	5863							-8.8	-8.8	-10.5	0.00%	0.00%	0.00%
Cefaclor		5575-21-3	5575213	5241	PharmaUBA	5864	4.80	1.27	3				-8.3	-8.8	-10.8	0.00%	0.00%	0.00%
Dexpanthenol		81-13-0	81130	3802	Reach_272	5865							-8.4	-8.8	-10.8	0.00%	0.00%	0.00%
IMATINIB		152459-95-5	152459955	2024	PharmaBeta_332	5866							-8.8	-8.8	-10.8	0.00%	0.00%	0.00%
Nebivolol		99200-09-6	99200096	5062	PharmaBeta_542	5867							-8.8	-8.8	-10.8	0.00%	0.00%	0.00%
Almotriptan		177036-94-1	177036941	4835	PharmaBeta_25	5868							-8.8	-8.8	-10.6	0.00%	0.00%	0.00%
CINACALCET		226256-56-0	226256560	4876	PharmaBeta_132	5869							-8.7	-8.8	-10.4	0.00%	0.00%	0.00%
Fenoprofen		13392-18-2	13392182	5310	PharmaUBA	5870							-9.1	-8.8	-10.9	0.00%	0.00%	0.00%
Zolmitriptan		139264-17-8	139264178	1918	PharmaBeta_800	5871							-8.8	-8.8	-10.6	0.00%	0.00%	0.00%
MECLOZINE		569-65-3	569653	3218	PharmaBeta_476	5872	1.94	0.15	3				-9.1	-8.9	-10.4	0.00%	0.00%	0.00%
FLUPENTIXOL		2709-56-0	2709560	2495	PharmaBeta_269	5873							-9.0	-8.9	-10.4	0.00%	0.00%	0.00%
Torasemide		56211-40-6	56211406	5165	PharmaBeta_754	5874							-9.0	-9.0	-10.7	0.00%	0.00%	0.00%
Moxifloxacin		354812-41-2	354812412	2017	PharmaBeta_519	5875							-8.7	-9.0	-11.0	0.00%	0.00%	0.00%
DESMOPRESSIN		16679-58-6	16679586	6397	PharmaBeta_159	5876							-9.2	-9.0	-10.5	0.00%	0.00%	0.00%
Rizatriptan		162401-32-3	162401323	5123	PharmaBeta_664	5877							-8.8	-9.0	-11.1	0.00%	0.00%	0.00%
Tacrolimus		104987-11-3	104987113	5455	PharmaUBA	5878							-9.3	-9.0	-11.1	0.00%	0.00%	0.00%
Famciclovir		58306-30-2	58306302	5307	PharmaUBA	5879	3.64	0.59	3				-8.6	-9.0	-11.1	0.00%	0.00%	0.00%
GOSERELIN		65807-02-5	65807025	6403	PharmaBeta_309	5880							-9.2	-9.0	-10.5	0.00%	0.00%	0.00%
Saxagliptin		28523-86-6	28523866	5131	PharmaBeta_680	5881							-8.8	-9.1	-11.1	0.00%	0.00%	0.00%
Lamivudine		134678-17-4	134678174	1881	PharmaBeta_427	5882	4.35	1.14	3				-8.6	-9.1	-11.1	0.00%	0.00%	0.00%
Nalidixic Acid		389-08-2	389082	5376	PharmaUBA	5883							-9.1	-9.1	-11.1	0.00%	0.00%	0.00%
Capsaicin		404-86-4	404864	627	PharmaBeta_114	5884							-9.2	-9.1	-10.8	0.00%	0.00%	0.00%
Tibolone		5630-53-5	5630535	3189	PharmaBeta_735	5885							-9.2	-9.1	-10.8	0.00%	0.00%	0.00%
Agomelatine		56180-94-0	56180940	4831	PharmaBeta_13	5886							-9.1	-9.1	-11.2	0.00%	0.00%	0.00%
Retigabine		155213-67-5	155213675	5121	PharmaBeta_653	5887							-9.2	-9.1	-11.2	0.00%	0.00%	0.00%
Prasterone		53-43-0	53430	3101	Reach_20	5888							-9.2	-9.1	-10.9	0.00%	0.00%	0.00%
TERAZOSIN		63590-64-7	63590647	3413	PharmaBeta_725	5889							-8.9	-9.1	-11.2	0.00%	0.00%	0.00%
Pindolol		137-58-6	137586	23	PharmaBeta_609	5890							-9.2	-9.1	-10.7	0.00%	0.00%	0.00%
Praziquantel		31218-83-4	31218834	1159	PharmaUBA	5891							-9.3	-9.1	-10.4	0.00%	0.00%	0.00%
TAPENTADOL		175591-23-8	175591238	5142	PharmaBeta_715	5892							-9.4	-9.1	-11.2	0.00%	0.00%	0.00%
Dutasteride		496775-61-2	496775612	4918	PharmaBeta_194	5893							-9.1	-9.1	-10.9	0.00%	0.00%	0.00%
Tetrabenazine		58-46-8	58468	5154	PharmaBeta_730	5894							-9.3	-9.2	-11.2	0.00%	0.00%	0.00%
Desogestrel		54024-22-5	54024225	3117	PharmaBeta_160	5895							-9.2	-9.2	-10.9	0.00%	0.00%	0.00%
Perphenazine		58-39-9	58399	3246	PharmaBeta_603	5896							-9.2	-9.2	-11.2	0.00%	0.00%	0.00%
Caffeine		58-08-2	58082	66	Reach_45	5897							-9.3	-9.2	-10.1	0.00%	0.00%	0.00%
Diethylstilbestrol		128-46-1	128461	1133	PharmaUBA	5898							-9.1	-9.2	-10.4	0.00%	0.00%	0.00%
Rotigotine		106308-44-5	106308445	5127	PharmaBeta_671	5899							-9.2	-9.2	-11.0	0.00%	0.00%	0.00%
Lanreotide		129805-33-0	129805330	6462	PharmaBeta_429	5900							-9.4	-9.3	-10.7	0.00%	0.00%	0.00%
Piperazine		110-85-0	110850	1531	Reach_832	5901							-9.4	-9.3	-11.3	0.00%	0.00%	0.00%
Mesterolone		1424-00-6	1424006	1955	Reach_1679	5902							-9.4	-9.3	-11.1	0.00%	0.00%	0.00%
Triptorelin		7722-84-1	7722841	6451	PharmaBeta_766	5903							-9.5	-9.3	-10.8	0.00%	0.00%	0.00%
Buprenorphine		52485-79-7	52485797	3061	PharmaBeta_107	5904							-9.3	-9.4	-11.4	0.00%	0.00%	0.00%
Estriol		50-27-1	50271	54	PharmaBeta_225	5905							-9.5	-9.4	-10.8	0.00%	0.00%	0.00%
Prasugrel		81093-37-0	81093370	5100	PharmaBeta_622	5906							-9.4	-9.4	-11.5	0.00%	0.00%	0.00%
Minoxidil		38304-91-5	38304915	2820	PharmaBeta_508	5907							-9.1	-9.4	-11.5	0.00%	0.00%	0.00%
Triamcinolone Acetonide		76-25-5	76255	5469	PharmaUBA	5908							-9.4	-9.5	-11.5	0.00%	0.00%	0.00%
Eletriptan		143322-58-1	143322581	1963	PharmaBeta_199	5909							-9.4	-9.5	-11.5	0.00%	0.00%	0.00%
Zidovudine		30516-87-1	30516871	2602	PharmaBeta_796	5910							-9.0	-9.5	-11.5	0.00%	0.00%	0.00%
Phenylephrine Hydrochloride		61-76-7	61767	5952	Reach_60	5911							-9.7	-9.5	-11.0	0.00%	0.00%	0.00%
Tenoxicam		59804-37-4	59804374	5459	PharmaUBA	5912							-9.4	-9.5	-11.6	0.00%	0.00%	0.00%
Guaifenesin		93-14-1	93141	4061	PharmaBeta_312	5913							-9.3	-9.5	-11.6	0.00%	0.00%	0.00%
Melatonin		73-31-4	73314	3619	PharmaBeta_477	5914							-9.4	-9.5	-11.6	0.00%	0.00%	0.00%
Pimecrolimus		111025-46-8	111025468	5096	PharmaBeta_608	5915							-9.7	-9.5	-11.5	0.00%	0.00%	0.00%
Rifaximin		19395-41-6	19395416	5429	PharmaUBA	5916							-9.1	-9.5	-10.7	0.00%	0.00%	0.00%
Atazanavir		198904-31-3	198904313	2244	PharmaBeta_57	5917							-9.6	-9.6	-11.3	0.00%	0.00%	0.00%
Acitretin		55079-83-9	55079839	3159	PharmaBeta_9	5918							-9.2	-9.6	-10.9	0.00%	0.00%	0.00%
Etonogestrel		54048-10-1	54048101	3119	PharmaBeta_229	5919							-9.7	-9.6	-11.3	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Pyrimethamine		58-14-0	58140	1161	PharmaUBA	5920							-9.8	-9.6	-10.5	0.00%	0.00%	0.00%
Deferiprone		51146-56-6	51146566	4890	PharmaBeta_154	5921							-9.2	-9.6	-11.7	0.00%	0.00%	0.00%
Acrivastine		87848-99-5	87848995	5218	PharmaUBA	5922							-9.4	-9.6	-11.7	0.00%	0.00%	0.00%
Alfentanil		71195-58-9	71195589	3578	PharmaBeta_19	5923							-9.6	-9.6	-11.4	0.00%	0.00%	0.00%
Glimepiride		93479-97-1	93479971	4070	PharmaBeta_302	5924							-9.6	-9.7	-11.6	0.00%	0.00%	0.00%
Probenecid		57-66-9	57669	3237	PharmaBeta_628	5925							-9.5	-9.7	-11.7	0.00%	0.00%	0.00%
Darunavir		302962-49-8	302962498	4887	PharmaBeta_150	5926							-9.6	-9.7	-11.8	0.00%	0.00%	0.00%
Benzyl Benzoate		120-51-4	120514	359	Reach_996	5927							-10.0	-9.7	-11.6	0.00%	0.00%	0.00%
Isotretinoin		154-21-2	154212	1146	PharmaUBA	5928							-9.2	-9.8	-10.8	0.00%	0.00%	0.00%
Nimodipine		104206-65-7	104206657	5068	PharmaBeta_554	5929							-9.8	-9.8	-11.8	0.00%	0.00%	0.00%
Efavirenz		154598-52-4	154598524	2038	PharmaBeta_196	5930							-9.9	-9.8	-11.6	0.00%	0.00%	0.00%
Betaxolol		63659-18-7	63659187	4850	PharmaBeta_87	5931							-9.8	-9.8	-11.9	0.00%	0.00%	0.00%
Repaglinide		135062-02-1	135062021	1886	PharmaBeta_651	5932							-9.7	-9.9	-11.6	0.00%	0.00%	0.00%
Cefpodoxime		82619-04-3	82619043	5250	PharmaUBA	5933							-9.7	-9.9	-12.0	0.00%	0.00%	0.00%
Glucagon		76712-82-8	76712828	6429	PharmaBeta_304	5934							-10.1	-9.9	-11.4	0.00%	0.00%	0.00%
Benzoic Acid		65-85-0	65850	785	Reach_77	5935							-10.2	-9.9	-12.0	0.00%	0.00%	0.00%
Bromocriptine		25614-03-3	25614033	5232	PharmaUBA	5936							-9.9	-10.0	-12.0	0.00%	0.00%	0.00%
Cilazapril		88768-40-5	88768405	5515	PharmaUBA	5937							-9.9	-10.0	-12.0	0.00%	0.00%	0.00%
Fluticasone		90566-53-3	90566533	4002	PharmaBeta_271	5938							-9.9	-10.0	-12.0	0.00%	0.00%	0.00%
Diflunisal		125-28-0	125280	5282	PharmaUBA	5939							-10.1	-10.1	-12.1	0.00%	0.00%	0.00%
Rifabutin		72559-06-9	72559069	3606	PharmaBeta_655	5940							-9.8	-10.2	-11.5	0.00%	0.00%	0.00%
Fenbufen		31879-05-7	31879057	5309	PharmaUBA	5941							-10.2	-10.2	-11.9	0.00%	0.00%	0.00%
Degarelix		214766-78-6	214766786	6424	PharmaBeta_156	5942							-10.4	-10.2	-11.7	0.00%	0.00%	0.00%
Hyoscine		51-34-3	51343	3036	Reach_15	5943							-9.9	-10.2	-12.2	0.00%	0.00%	0.00%
Pirenzepine		79548-73-5	79548735	5415	PharmaUBA	5944							-10.2	-10.2	-12.3	0.00%	0.00%	0.00%
Isradipine		155974-00-8	155974008	4985	PharmaBeta_350	5945							-10.3	-10.2	-12.3	0.00%	0.00%	0.00%
Thalidomide		175591-23-8	175591238	5141	PharmaBeta_713	5946							-9.9	-10.3	-12.3	0.00%	0.00%	0.00%
Fentanyl		437-38-7	437387	2914	PharmaBeta_247	5947							-10.3	-10.3	-12.3	0.00%	0.00%	0.00%
Metolazone		13265-10-6	13265106	5033	PharmaBeta_490	5948							-10.0	-10.4	-12.5	0.00%	0.00%	0.00%
Sirolimus		53123-88-9	53123889	3089	PharmaBeta_690	5949							-10.6	-10.4	-12.4	0.00%	0.00%	0.00%
Bimatoprost		155206-00-1	155206001	4852	PharmaBeta_93	5950							-10.4	-10.4	-12.4	0.00%	0.00%	0.00%
Fluocortolone		152-97-6	152976	2026	Reach_1209	5951							-10.4	-10.4	-12.5	0.00%	0.00%	0.00%
KETOTIFEN		10596-23-3	10596233	4991	PharmaBeta_386	5952							-10.5	-10.5	-12.5	0.00%	0.00%	0.00%
Thioridazine		55297-95-5	55297955	5460	PharmaUBA	5953							-10.3	-10.5	-12.1	0.00%	0.00%	0.00%
Raltegravir		132875-61-7	132875617	5118	PharmaBeta_645	5954							-10.2	-10.5	-12.6	0.00%	0.00%	0.00%
Tocofersolan		9002-96-4	9002964	5162	PharmaBeta_748	5955							-10.8	-10.6	-11.3	0.00%	0.00%	0.00%
Acetic Acid		64-19-7	64197	778	Reach_72	5956							-10.9	-10.7	-12.6	0.00%	0.00%	0.00%
Phenol		108-95-2	108952	252	Reach_765	5957							-11.2	-10.9	-12.8	0.00%	0.00%	0.00%
Latanoprost		191732-72-6	191732726	5004	PharmaBeta_434	5958							-10.8	-10.9	-12.8	0.00%	0.00%	0.00%
Fulvestrant		129453-61-8	129453618	414	PharmaBeta_283	5959							-11.2	-11.0	-11.6	0.00%	0.00%	0.00%
Benperidol		983-42-6	983426	5506	PharmaUBA	5960							-11.0	-11.0	-13.1	0.00%	0.00%	0.00%
Prednisone		53-03-2	53032	5102	PharmaBeta_625	5961							-11.0	-11.0	-13.1	0.00%	0.00%	0.00%
Misoprostol		59122-46-2	59122462	3267	PharmaBeta_510	5962							-11.0	-11.0	-13.0	0.00%	0.00%	0.00%
Tretinoin		57-91-0	57910	1117	PharmaBeta_760	5963							-10.5	-11.1	-12.1	0.00%	0.00%	0.00%
Alprostadil		745-65-3	745653	3640	PharmaBeta_27	5964							-11.1	-11.1	-13.1	0.00%	0.00%	0.00%
Salmeterol		62989-33-7	62989337	5129	PharmaBeta_678	5965							-11.2	-11.2	-13.2	0.00%	0.00%	0.00%
Penciclovir		97825-25-7	97825257	5552	PharmaUBA	5966							-10.8	-11.3	-13.3	0.00%	0.00%	0.00%
Fluocinonide		356-12-7	356127	5317	PharmaUBA	5967							-11.1	-11.3	-13.4	0.00%	0.00%	0.00%
Erlotinib		183321-74-6	183321746	2183	PharmaBeta_216	5968							-11.3	-11.3	-13.4	0.00%	0.00%	0.00%
Mesna		19767-45-4	19767454	5019	PharmaBeta_485	5969							-10.7	-11.4	-13.2	0.00%	0.00%	0.00%
Paliperidone		58-74-2	58742	5083	PharmaBeta_588	5970							-11.1	-11.4	-13.5	0.00%	0.00%	0.00%
Roflumilast		91374-21-9	91374219	5124	PharmaBeta_665	5971							-11.6	-11.5	-13.6	0.00%	0.00%	0.00%
Flunisolide		3385-03-3	3385033	5315	PharmaUBA	5972							-11.5	-11.6	-13.6	0.00%	0.00%	0.00%
Phenylbutazone		50-33-9	50339	5412	PharmaUBA	5973							-11.4	-11.6	-13.6	0.00%	0.00%	0.00%
Nitisinone		58691-88-6	58691886	5069	PharmaBeta_555	5974							-11.6	-11.6	-13.7	0.00%	0.00%	0.00%
Travoprost		81846-19-7	81846197	5172	PharmaBeta_758	5975							-11.5	-11.7	-13.6	0.00%	0.00%	0.00%
Busulfan		55-98-1	55981	708	PharmaBeta_110	5976							-11.4	-11.7	-13.7	0.00%	0.00%	0.00%
Aprepitant		170729-80-3	170729803	2120	PharmaBeta_53	5977							-11.9	-11.9	-14.0	0.00%	0.00%	0.00%
Entecavir		142217-69-4	142217694	4922	PharmaBeta_205	5978							-11.6	-12.0	-14.1	0.00%	0.00%	0.00%
Dydrogesterone		152-62-5	152625	5293	PharmaUBA	5979							-12.2	-12.0	-14.1	0.00%	0.00%	0.00%
Ivermectin		16846-24-5	16846245	5343	PharmaUBA	5980							-12.2	-12.1	-14.1	0.00%	0.00%	0.00%
Everolimus		159351-69-6	159351696	2068	PharmaBeta_235	5981							-12.3	-12.1	-14.1	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'						
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]		TP(Cwcoast) [-]
Fumaric Acid		110-17-8	110178	276	Reach_807	5982							-11.6	-12.2	-14.3	0.00%	0.00%		0.00%
NAFARELIN		83150-76-9	83150769	6440	PharmaBeta_525	5983							-12.4	-12.2	-13.7	0.00%	0.00%		0.00%
Tafluprost		50-35-1	50351	5140	PharmaBeta_711	5984							-12.1	-12.3	-13.9	0.00%	0.00%		0.00%
Zanamivir		139110-80-8	139110808	1916	PharmaBeta_795	5985							-11.7	-12.4	-14.4	0.00%	0.00%		0.00%
Triamcinolone		124-94-7	124947	1795	PharmaBeta_761	5986							-12.4	-12.5	-14.6	0.00%	0.00%		0.00%
Nepafenac		54-11-5	54115	5066	PharmaBeta_546	5987							-12.5	-12.7	-14.7	0.00%	0.00%		0.00%
Cetrorelix		120287-85-6	120287856	6418	PharmaBeta_126	5988							-13.0	-12.8	-14.3	0.00%	0.00%		0.00%
Flumazenil		78755-81-4	78755814	4957	PharmaBeta_262	5989							-13.1	-13.3	-15.3	0.00%	0.00%		0.00%
NANDROLONE		437-38-7	437387	2914	PharmaBeta_247	5990							-14.3	-14.3	-16.3	0.00%	0.00%		0.00%
Metronidazole		443-48-1	443481	642	PharmaBeta_493	5991	5.36	0.61	10	4.99	0.70								
Ciprofloxacin		86386-73-4	86386734	969	PharmaBeta_135	5992	4.79	0.37	3	3.79	0.37								
Tobramycin		32986-56-4	32986564	2672	PharmaBeta_747	5993													
Amikacin		37517-28-5	37517285	2801	PharmaBeta_36	5994													
Tigecycline		69004-04-2	69004042	5559	PharmaUBA	5995													
Pesticides																			
count							*411*	*399*	*411*	*363*	*363*	*170*	*420*	*420*	*420*	*420*	*420*	*2.1%*	*420*
sum																*0.9%*	*0.7%*	*97.8%*	*0.003%*
standard deviation							*1.26*	*0.43*		*1.31*	*0.46*		*1.0*	*1.0*	*1.0*				
2.5-p													*-7.7*	*-7.9*	*-9.2*	*4.7E-15*	*1.2E-15*		*1.7E-20*
50-p							*3.35*	*0.93*	*11*	*2.12*	*0.97*	*9*	*-5.8*	*-6.0*	*-7.0*	*4.0E-09*	*9.5E-10*		*1.4E-12*
97.5-p													*-4.1*	*-4.2*	*-5.4*	*1.9E-05*	*1.5E-05*		*3.0E-08*
Sulphur		7704-34-9	7704349	6446	Pest_418	5997	5.83	0.56	8	4.83	0.56		-2.7	-2.6	-4.1	0.39%	0.44%	0.436%	0.00%
Mancozeb		8018-01-7	8018017	1185	Pest_242	5998	3.12	0.63	15	1.05	0.47	3	-3.1	-3.1	-4.5	0.09%	0.10%	0.531%	0.00%
Glyphosate		1071-83-6	1071836	212	Pest_15	5999	4.63	0.88	36	3.46	0.93	22	-2.8	-3.2	-5.1	0.23%	0.06%	0.591%	0.00%
Chlormequat		7003-89-6	7003896	4871	Pest_302	6000	5.12	0.63	6	4.12	0.63		-3.1	-3.4	-5.2	0.09%	0.03%	0.622%	0.00%
Isoproturon		34123-59-6	34123596	49	Pest_157	6001	2.94	1.40	34	1.04	0.22	8	-3.6	-3.6	-4.4	0.02%	0.02%	0.638%	0.00%
Metiram		9006-42-2	9006422	6288	Pest_377	6002	2.92	1.39	16	1.40	0.87	33	-3.7	-3.7	-5.1	0.01%	0.01%	0.649%	0.00%
Atrazine		1912-24-9	1912249	37	Reach_1734	6003	3.28	1.13	134	1.95	0.98	95	-4.0	-3.9	-5.4	0.00%	0.00%	0.653%	0.00%
Copper oxychloride		1332-40-7	1332407	6252	Pest_310	6004	3.16	1.17	13	2.16	0.69	52	-4.0	-3.9	-5.4	0.00%	0.00%	0.657%	0.00%
Terbuthylazine		5915-41-3	5915413	70	Pest_201	6005	3.32	1.16	17	0.61	0.53	8	-4.0	-4.0	-5.4	0.00%	0.00%	0.661%	0.00%
Ziram		137-30-4	137304	6353	Pest_436	6006	2.55	0.75	20	1.86	0.69	9	-4.1	-4.1	-5.5	0.00%	0.00%		0.00%
Metazachlor		67129-08-2	67129082	81	Pest_215	6007	3.80	1.04	6	2.80	0.80		-3.9	-4.2	-5.3	0.00%	0.00%		0.00%
Chloridazon		1698-60-8	1698608	35	Pest_93	6008	4.30	1.04	8	2.54	0.73		-4.2	-4.2	-5.6	0.00%	0.00%		0.00%
Propineb		12071-83-9	12071839	6443	Pest_402	6009							-4.3	-4.2	-5.7	0.00%	0.00%		0.00%
Copper		7440-50-8	7440508	6419	Pest_305	6010	2.26	0.70	74	1.34	0.45	15	-4.3	-4.3	-5.7	0.00%	0.00%		0.00%
2,4-D		94-75-7	94757	111	Pest_278	6011	4.71	0.93	51	3.65	1.04	23	-4.2	-4.4	-5.4	0.00%	0.00%		0.00%
MCPA		94-74-6	94746	110	Pest_369	6012	4.46	1.11	22	3.88	1.23	8	-4.5	-4.4	-5.3	0.00%	0.00%		0.00%
Dimethomorph		110488-70-5	110488705	4906	Pest_330	6013	4.19	0.38	12	2.74	0.46	3	-4.1	-4.5	-5.8	0.00%	0.00%		0.00%
Thiram		137-26-8	137268	441	Reach_1137	6014	2.18	1.10	36	1.11	1.00	7	-4.3	-4.5	-5.4	0.00%	0.00%		0.00%
Acetochlor		34256-82-1	34256821	608	Pest_158	6015	3.22	0.68	12	1.93	1.22	10	-4.3	-4.5	-5.5	0.00%	0.00%		0.00%
Metamitron		41394-05-2	41394052	632	Pest_173	6016	5.33	0.28	4	4.33	0.28		-4.5	-4.5	-5.9	0.00%	0.00%		0.00%
Copper sulphate		7758-98-7	7758987	6253	Pest_312	6017	2.41	0.82	271	1.37	0.52	28	-4.5	-4.5	-5.9	0.00%	0.00%		0.00%
Prometryn		7287-19-6	7287196	87	Pest_228	6018	3.03	1.08	23	1.26	1.39	8	-4.6	-4.5	-6.0	0.00%	0.00%		0.00%
Propachlor		1918-16-7	1918167	520	Pest_107	6019	2.99	0.90	10	1.66	0.93		-4.6	-4.5	-6.0	0.00%	0.00%		0.00%
Imidacloprid		138261-41-3	138261413	443	Pest_68	6020	2.95	1.78	37	1.60	1.34	10	-4.2	-4.5	-5.8	0.00%	0.00%		0.00%
Maneb		12427-38-2	12427382	6283	Pest_368	6021	3.34	1.13	36	1.44	0.43	3	-4.6	-4.6	-6.0	0.00%	0.00%		0.00%
Zineb		12122-67-7	12122677	6453	Pest_435	6022	4.37	0.92	23	3.37	0.87	69	-4.6	-4.6	-6.0	0.00%	0.00%		0.00%
Glufosinate		51276-47-2	51276472	4969	Pest_359	6023	3.76	1.01	6	2.76	1.01		-4.1	-4.6	-6.6	0.00%	0.00%		0.00%
Captan		133-06-2	133062	425	Pest_58	6024	2.53	0.74	32	2.83	1.63	6	-4.2	-4.6	-5.9	0.00%	0.00%		0.00%
Azoxystrobin		131860-33-8	131860338	423	Pest_56	6025	2.65	0.47	19	1.88	0.98	19	-4.3	-4.7	-6.0	0.00%	0.00%		0.00%
Alachlor		15972-60-8	15972608	497	Pest_86	6026	3.51	0.72	29	1.59	1.26	8	-4.7	-4.7	-5.8	0.00%	0.00%		0.00%
Fosetyl		15845-66-6	15845666	4965	Pest_358	6027	6.36	1.01	3				-4.7	-4.7	-6.9	0.00%	0.00%		0.00%
Pyrazophos		13457-18-6	13457186	432	Pest_62	6028	3.14	1.24	13	2.14	1.38	39	-4.8	-4.7	-6.2	0.00%	0.00%		0.00%
Iprodione		36734-19-7	36734197	616	Pest_163	6029	3.48	0.45	10	1.95	0.53		-4.8	-4.7	-6.2	0.00%	0.00%		0.00%
Dimethenamid-P		163515-14-8	163515148	502	Pest_88	6030	3.89	0.63	15	1.56	0.17		-4.8	-4.7	-6.2	0.00%	0.00%		0.00%
Dimethoate		60-51-5	60515	753	Pest_204	6031	3.31	1.35	82	3.42	1.29	21	-4.8	-4.7	-6.2	0.00%	0.00%		0.00%
Copper oxide		1317-38-0	1317380	6421	Pest_309	6032	3.60	0.94	6	1.14	0.40		-4.8	-4.7	-6.2	0.00%	0.00%		0.00%
Copper hydroxide		20427-59-2	20427592	6420	Pest_308	6033	3.17	0.65	12	1.35	0.39	3	-4.8	-4.7	-6.2	0.00%	0.00%		0.00%
Oxine-copper		10380-28-6	10380286	6302	Pest_389	6034	2.57	1.06	11	0.62	0.61	5	-4.8	-4.7	-6.2	0.00%	0.00%		0.00%
Copper carbonate		1184-64-1	1184641	6251	Pest_306	6035							-4.8	-4.7	-6.2	0.00%	0.00%		0.00%
Cyanazine		21725-46-2	21725462	535	Pest_116	6036	3.73	0.99	18	1.04	0.74	11	-4.8	-4.8	-6.2	0.00%	0.00%		0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Epoxyconazole		133855-98-8	133855988	4924	Pest_338	6037	3.29	0.88	8	1.73	1.08		-4.6	-4.8	-5.7	0.00%	0.00%	0.00%
Dodine		2439-10-3	2439103	6262	Pest_336	6038	3.05	0.89	17	0.90	1.17	4	-4.9	-4.8	-6.3	0.00%	0.00%	0.00%
Triflumizole		68694-11-1	68694111	802	Pest_219	6039	2.99	0.46	13	2.14	0.38	3	-5.0	-4.8	-5.7	0.00%	0.00%	0.00%
Methomyl		16752-77-5	16752775	506	Pest_90	6040	2.73	0.79	49	1.75	1.04	4	-5.0	-4.8	-6.1	0.00%	0.00%	0.00%
Dimethachlor		50563-36-5	50563365	663	Pest_179	6041	3.63	0.77	6	2.63	0.80		-5.0	-4.8	-6.0	0.00%	0.00%	0.00%
Difenzoquat		49866-87-7	49866877	4903	Pest_326	6042	4.26	1.50	4	3.26	1.12		-5.1	-4.9	-6.2	0.00%	0.00%	0.00%
Oxamyl		23135-22-0	23135220	549	Pest_124	6043	3.41	0.62	15	2.81	1.13	9	-4.6	-4.9	-6.4	0.00%	0.00%	0.00%
Metribuzin		21087-64-9	21087649	531	Pest_113	6044	4.05	1.03	16	1.82	1.36	12	-4.5	-4.9	-5.8	0.00%	0.00%	0.00%
Paraquat		4685-14-7	4685147	5085	Pest_391	6045	3.86	1.08	29	2.86	1.12	29	-4.7	-4.9	-6.6	0.00%	0.00%	0.00%
Thiacloprid		111988-49-9	111988499	6	Pest_20	6046	3.27	1.51	15	2.32	1.66	6	-4.5	-4.9	-5.8	0.00%	0.00%	0.00%
Carbendazim		10605-21-7	10605217	3	Pest_299	6047	3.53	1.22	29	2.85	1.14	6	-4.4	-4.9	-5.7	0.00%	0.00%	0.00%
Bentazone		25057-89-0	25057890	39	Pest_290	6048	5.12	0.59	11	2.46	1.12	7	-4.5	-4.9	-6.3	0.00%	0.00%	0.00%
Trichlorfon		52-68-6	52686	677	Pest_183	6049	2.86	1.41	84	1.98	2.84	5	-4.6	-4.9	-6.0	0.00%	0.00%	0.00%
Folpet		133-07-3	133073	426	Pest_59	6050	2.75	1.00	27	1.75	0.84	27	-4.3	-4.9	-6.1	0.00%	0.00%	0.00%
Dicloran		99-30-9	99309	1085	Pest_276	6051	3.82	0.82	8	2.82	0.84		-4.8	-4.9	-5.7	0.00%	0.00%	0.00%
Propyzamide		23950-58-5	23950585	556	Pest_128	6052	4.50	0.74	11	2.85	0.47	8	-4.9	-4.9	-5.9	0.00%	0.00%	0.00%
Chlorothalonil		1897-45-6	1897456	516	Pest_102	6053	2.01	0.74	66	0.90	1.42	29	-5.1	-4.9	-5.6	0.00%	0.00%	0.00%
Thiabendazole		148-79-8	148798	476	Pest_77	6054	3.53	0.77	10	1.49	1.07		-4.5	-5.0	-5.8	0.00%	0.00%	0.00%
Diquat		2764-72-9	2764729	4912	Pest_334	6055	3.50	1.22	32	2.50	1.12	32	-4.8	-5.0	-7.1	0.00%	0.00%	0.00%
Thiophanate-methyl		23564-05-8	23564058	552	Pest_126	6056	4.00	0.72	20	3.08	0.65	7	-4.6	-5.0	-5.9	0.00%	0.00%	0.00%
Ethofumesate		26225-79-6	26225796	573	Pest_136	6057	4.35	0.71	10	3.29	0.46		-4.9	-5.0	-6.2	0.00%	0.00%	0.00%
Flutriafol		76674-21-0	76674210	875	Pest_236	6058	4.06	0.74	15	3.47	0.69	4	-4.6	-5.1	-5.8	0.00%	0.00%	0.00%
Aclonifen		74070-46-5	74070465	835	Pest_233	6059	2.29	1.03	8	0.60	0.48		-5.0	-5.1	-5.7	0.00%	0.00%	0.00%
Oryzalin		19044-88-3	19044883	517	Pest_103	6060	2.84	0.74	9	1.54	0.83		-4.6	-5.1	-6.0	0.00%	0.00%	0.00%
Mecoprop-P		16484-77-8	16484778	503	Reach_2421	6061	4.90	0.76	9	4.67	0.13		-5.2	-5.1	-5.6	0.00%	0.00%	0.00%
S-Metolachlor		87392-12-9	87392129	1115	Pest_411	6062	3.66	1.04	8	1.90	1.31		-5.1	-5.1	-5.8	0.00%	0.00%	0.00%
Vamidothion		2275-23-2	2275232	543	Pest_119	6063	4.74	2.15	3	3.74	1.38		-4.8	-5.1	-6.2	0.00%	0.00%	0.00%
Chlorthal		2136-79-0	2136790	4873	Pest_303	6064	2.82	0.24	3				-4.8	-5.1	-6.4	0.00%	0.00%	0.00%
Flumetsulam		98967-40-9	98967409	1081	Reach_4516	6065	4.42	2.08	12	3.42	2.08		-4.6	-5.1	-5.9	0.00%	0.00%	0.00%
Phenmedipham		13684-63-4	13684634	440	Pest_66	6066	3.93	0.56	11	2.93	0.56	11	-5.0	-5.1	-5.9	0.00%	0.00%	0.00%
Flufenacet		142459-58-3	142459583	461	Pest_73	6067	3.59	0.25	6	1.97	1.42		-5.2	-5.1	-6.0	0.00%	0.00%	0.00%
Bromofenoxim		13181-17-4	13181174	422	Pest_55	6068	2.73	0.52	9	1.73	0.52		-4.5	-5.1	-6.2	0.00%	0.00%	0.00%
Sulcotrione		99105-77-8	99105778	1083	Pest_274	6069	4.16	1.52	5	1.74	1.44		-4.6	-5.2	-6.6	0.00%	0.00%	0.00%
1,3-Dichloropropene		542-75-6	542756	1107	Pest_277	6070	3.39	0.51	20	2.80	1.14	6	-5.6	-5.2	-6.8	0.00%	0.00%	0.00%
Fluquinconazole		136426-54-5	136426545	438	Pest_64	6071	2.82	0.75	5	2.70	0.19		-4.7	-5.2	-6.1	0.00%	0.00%	0.00%
Mesotrione		104206-82-8	104206828	167	Pest_13	6072	5.03	0.85	6	3.64	1.48		-4.7	-5.2	-6.8	0.00%	0.00%	0.00%
Dichlobenil		1194-65-6	1194656	352	Reach_1672	6073	3.97	0.58	51	2.55	0.76	10	-5.3	-5.2	-5.9	0.00%	0.00%	0.00%
Methamidophos		10265-92-6	10265926	153	Pest_9	6074	3.79	1.10	18	2.79	1.10	18	-5.3	-5.2	-6.1	0.00%	0.00%	0.00%
Heptenophos		23560-59-0	23560590	551	Pest_125	6075	2.15	1.94	5	1.15	1.01		-5.4	-5.2	-6.4	0.00%	0.00%	0.00%
Pendimethalin		40487-42-1	40487421	628	Pest_170	6076	2.98	1.07	31	1.73	1.46	19	-5.3	-5.2	-5.7	0.00%	0.00%	0.00%
DNOC		534-52-1	534521	682	Reach_1332	6077	3.11	0.54	12	3.05	0.74	14	-4.8	-5.2	-6.0	0.00%	0.00%	0.00%
Fluazinam		79622-59-6	79622596	925	Pest_240	6078	2.04	0.75	26	1.57	0.71	37	-5.3	-5.2	-5.9	0.00%	0.00%	0.00%
Simazine		122-34-9	122349	15	Pest_43	6079	3.88	1.16	56	2.24	1.16	23	-5.3	-5.2	-5.9	0.00%	0.00%	0.00%
Nuarimol		63284-71-9	63284719	773	Pest_207	6080	3.78	0.83	4	2.78	0.83		-4.8	-5.2	-6.0	0.00%	0.00%	0.00%
Mecoprop		93-65-2	93652	108	Pest_264	6081	4.67	0.58	3	3.67	0.76		-5.3	-5.2	-5.7	0.00%	0.00%	0.00%
Acephate		30560-19-1	30560191	596	Pest_147	6082	5.07	0.89	38	1.59	1.86	3	-4.9	-5.2	-6.5	0.00%	0.00%	0.00%
Linuron		330-55-2	330552	602	Pest_150	6083	2.81	0.89	20	1.39	0.87	25	-5.2	-5.2	-6.0	0.00%	0.00%	0.00%
Omethoate		1113-02-6	1113026	295	Pest_18	6084	4.20	1.56	11	3.20	1.38	33	-4.9	-5.2	-6.6	0.00%	0.00%	0.00%
Chlorotoluron		15545-48-9	15545489	32	Pest_82	6085	4.01	1.31	16	3.01	1.02	48	-5.1	-5.2	-6.1	0.00%	0.00%	0.00%
Tebuconazole		107534-96-3	107534963	221	Pest_16	6086	3.48	0.59	13	2.27	0.79	15	-4.6	-5.2	-5.9	0.00%	0.00%	0.00%
Monuron		150-68-5	150685	482	Pest_80	6087	4.53	1.02	39	3.53	1.02		-5.1	-5.3	-6.1	0.00%	0.00%	0.00%
Propanil		709-98-8	709988	816	Pest_224	6088	3.86	0.44	34	1.20	0.77	9	-5.4	-5.3	-6.5	0.00%	0.00%	0.00%
Famoxadone		131807-57-3	131807573	421	Pest_54	6089	1.01	0.84	7	0.78	0.79		-5.3	-5.3	-6.7	0.00%	0.00%	0.00%
Benzthiazuron		1929-88-0	1929880	522	Pest_109	6090	5.89		1				-4.9	-5.3	-6.1	0.00%	0.00%	0.00%
Vinclozolin		50471-44-8	50471448	661	Pest_178	6091	3.89	0.63	13	2.73	0.80	6	-5.3	-5.3	-6.7	0.00%	0.00%	0.00%
Monocrotophos		6923-22-4	6923224	803	Pest_220	6092	3.63	1.06	25	2.63	1.01	75	-4.9	-5.3	-6.4	0.00%	0.00%	0.00%
Bitertanol		55179-31-2	55179312	693	Pest_187	6093	3.35	0.35	7	2.35	0.35		-4.7	-5.3	-6.1	0.00%	0.00%	0.00%
Dimethenamid		87674-68-8	87674688	1109	Pest_329	6094	3.52	0.63	8	1.52	1.12		-4.8	-5.3	-6.5	0.00%	0.00%	0.00%
Prosulfocarb		52888-80-9	52888809	60	Pest_184	6095	2.91	0.50	14	2.17	0.45	3	-5.4	-5.3	-6.3	0.00%	0.00%	0.00%
Florasulam		145701-23-1	145701231	473	Pest_75	6096	4.87	0.67	7	2.58	2.00		-4.8	-5.3	-6.0	0.00%	0.00%	0.00%
Monolinuron		1746-81-2	1746812	511	Pest_96	6097	3.51	1.64	8	2.51	1.02		-5.4	-5.3	-6.1	0.00%	0.00%	0.00%
Tolylfluanid		731-27-1	731271	827	Pest_229	6098	2.40	0.65	6	1.40	0.65		-5.4	-5.3	-6.0	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Metoxuron		19937-59-8	19937598	527	Pest_111	6099	5.06	1.19	10	4.06	1.02		-5.1	-5.3	-6.5	0.00%	0.00%	0.00%
Fenarimol		60168-88-9	60168889	747	Pest_202	6100	3.23	1.40	7	1.08	2.05		-4.9	-5.3	-6.1	0.00%	0.00%	0.00%
Dicamba		1918-00-9	1918009	519	Pest_106	6101	4.43	0.86	19	2.08	1.06	8	-5.3	-5.3	-6.5	0.00%	0.00%	0.00%
Fentin		668-34-8	668348	790	Pest_214	6102	1.04	1.43	44	-0.36	0.79	6	-5.4	-5.3	-6.8	0.00%	0.00%	0.00%
Fentin acetate		900-95-8	900958	6427	Pest_345	6103	0.81	1.05	12	-0.19	1.06	36	-5.4	-5.3	-6.8	0.00%	0.00%	0.00%
Barium Polysulfide		50864-67-0	50864670	6239	Pest_288	6104							-5.4	-5.3	-6.8	0.00%	0.00%	0.00%
Fenuron		101-42-8	101428	147	Pest_6	6105	5.03	0.92	3	4.03	1.02		-5.1	-5.3	-6.2	0.00%	0.00%	0.00%
Trifluralin		1582-09-8	1582098	496	Pest_85	6106	2.51	0.88	48	1.32	1.06	14	-5.4	-5.3	-5.8	0.00%	0.00%	0.00%
Fenbutatin-oxide		13356-08-6	13356086	6426	Pest_340	6107	1.19	0.80	14	1.56	1.66	3	-5.4	-5.3	-6.8	0.00%	0.00%	0.00%
Fluometuron		2164-17-2	2164172	534	Pest_115	6108	3.85	0.80	27	2.52	0.67	13	-5.5	-5.4	-6.2	0.00%	0.00%	0.00%
Metobromuron		3060-89-7	3060897	598	Pest_148	6109	4.64	1.02	30	3.64	1.02		-5.3	-5.4	-6.1	0.00%	0.00%	0.00%
Fuberidazole		3878-19-1	3878191	622	Pest_166	6110	3.79	0.41	3	2.79	0.41		-4.8	-5.4	-6.1	0.00%	0.00%	0.00%
Myclobutanil		88671-89-0	88671890	984	Pest_261	6111	3.42	0.69	48	2.95	0.34		-5.5	-5.4	-6.1	0.00%	0.00%	0.00%
Aldicarb		116-06-3	116063	342	Pest_29	6112	2.94	1.15	33	1.13	0.84	5	-5.6	-5.4	-6.5	0.00%	0.00%	0.00%
Quinmerac		90717-03-6	90717036	1003	Pest_262	6113	4.98	0.18	6	3.98	0.18		-4.9	-5.4	-6.5	0.00%	0.00%	0.00%
Benomyl		17804-35-2	17804352	513	Pest_98	6114	3.30	0.96	20	1.88	0.90	5	-4.8	-5.4	-6.5	0.00%	0.00%	0.00%
Bromuconazole		116255-48-2	116255482	343	Pest_30	6115	3.12	0.70	9	1.56	0.57		-5.5	-5.4	-6.1	0.00%	0.00%	0.00%
Methiocarb		2032-65-7	2032657	528	Pest_112	6116	2.36	1.09	23	1.36	1.07	69	-5.5	-5.4	-6.1	0.00%	0.00%	0.00%
Propazine		139-40-2	139402	446	Reach_1144	6117	4.00	1.05	10	1.82	0.87		-5.6	-5.4	-6.1	0.00%	0.00%	0.00%
Fentin hydroxide		76-87-9	76879	1110	Pest_346	6118	1.82	1.20	35	-0.68	0.75	4	-5.0	-5.4	-6.2	0.00%	0.00%	0.00%
Diuron		330-54-1	330541	46	Reach_1238	6119	2.82	1.26	86	1.27	1.02	23	-5.4	-5.4	-6.3	0.00%	0.00%	0.00%
Hexaconazole		79983-71-4	79983714	930	Pest_241	6120	3.40	0.69	68	2.29	0.69		-4.9	-5.5	-6.1	0.00%	0.00%	0.00%
Clopyralid		1702-17-6	1702176	509	Pest_94	6121	4.83	0.86	6	3.83	0.86		-5.5	-5.5	-6.4	0.00%	0.00%	0.00%
Pirimicarb		23103-98-2	23103982	547	Pest_123	6122	3.77	1.46	21	3.22	2.12	4	-5.5	-5.5	-6.4	0.00%	0.00%	0.00%
Fluroxypyr		69377-81-7	69377817	805	Pest_221	6123	4.60	0.85	33	3.60	0.85		-5.0	-5.5	-6.3	0.00%	0.00%	0.00%
Methabenzthiazuron		18691-97-9	18691979	515	Pest_100	6124	3.22	1.42	8	2.22	1.42		-5.1	-5.5	-6.6	0.00%	0.00%	0.00%
Fenfuram		24691-80-3	24691803	562	Pest_131	6125	4.04		1				-5.5	-5.5	-6.9	0.00%	0.00%	0.00%
Triadimenol		55219-65-3	55219653	694	Pest_188	6126	4.08	0.51	9	3.12	0.69		-4.8	-5.5	-6.1	0.00%	0.00%	0.00%
Napropamide		15299-99-7	15299997	5058	Pest_380	6127	4.00	0.63	36	1.95	1.08		-5.4	-5.5	-7.2	0.00%	0.00%	0.00%
Carbaryl		63-25-2	63252	76	Pest_206	6128	2.86	1.21	161	1.70	1.07	30	-5.7	-5.5	-6.5	0.00%	0.00%	0.00%
Triadimefon		43121-43-3	43121433	639	Pest_176	6129	3.83	0.50	10	2.66	0.76		-5.4	-5.5	-6.1	0.00%	0.00%	0.00%
Tebuthiuron		34014-18-1	34014181	607	Pest_156	6130	5.11	0.25	9	2.47	1.46		-5.1	-5.5	-6.6	0.00%	0.00%	0.00%
Dithianon		3347-22-6	3347226	604	Pest_153	6131	3.47	1.36	10	2.47	1.36		-4.7	-5.5	-6.1	0.00%	0.00%	0.00%
Triforine		26644-46-2	26644462	5180	Pest_433	6132	4.69	0.83	6	4.37	0.80		-5.2	-5.5	-6.6	0.00%	0.00%	0.00%
Boscalid		188425-85-6	188425856	36	Pest_101	6133	3.46	0.85	33	3.58	0.86		-5.1	-5.5	-6.7	0.00%	0.00%	0.00%
Alloxydim-sodium		55635-13-7	55635137	6234	Pest_286	6134	5.40	0.20	6	4.40	0.20		-5.6	-5.5	-7.0	0.00%	0.00%	0.00%
Diniconazole		83657-24-3	83657243	955	Pest_252	6135	3.83	0.61	3	2.83	0.69		-4.9	-5.5	-6.2	0.00%	0.00%	0.00%
Lenacil		2164-08-1	2164081	114	Pest_114	6136	3.61	1.56	5	2.61	1.56		-5.0	-5.5	-6.9	0.00%	0.00%	0.00%
Dichlorvos		62-73-7	62737	4897	Pest_324	6137	2.52	1.45	97	1.73	1.58	9	-5.8	-5.6	-7.0	0.00%	0.00%	0.00%
Flamprop-M		90134-59-1	90134591	4953	Pest_349	6138	3.20	0.62	3				-5.3	-5.6	-7.1	0.00%	0.00%	0.00%
Flamprop		58667-63-3	58667633	4952	Pest_348	6139	3.20	0.62	3				-5.3	-5.6	-7.1	0.00%	0.00%	0.00%
Terbumeton		33693-04-8	33693048	606	Pest_155	6140	4.28	0.27	5	3.28	0.27		-5.7	-5.6	-6.2	0.00%	0.00%	0.00%
Phosphamidon		13171-21-6	13171216	5093	Pest_394	6141	3.41	1.43	48	2.64	1.80	3	-5.4	-5.6	-7.2	0.00%	0.00%	0.00%
Demeton-S-methyl		919-86-8	919868	1010	Pest_263	6142	4.51	1.38	12	3.51	1.38		-5.7	-5.6	-6.4	0.00%	0.00%	0.00%
Dalapon		75-99-0	75990	4884	Pest_319	6143	5.60	0.89	19	4.60	0.89	19	-5.6	-5.6	-7.0	0.00%	0.00%	0.00%
Sodium-arsenite		7784-46-5	7784465	6328	Pest_415	6144	3.98	0.81	30	3.59	0.80	4	-5.6	-5.6	-7.0	0.00%	0.00%	0.00%
TCA		650-51-1	650511	1230	Reach_1486	6145	5.93	1.02	11	5.68	2.75	3	-5.6	-5.6	-7.0	0.00%	0.00%	0.00%
Naled		300-76-5	300765	594	Pest_145	6146	2.20	1.29	34	0.61	1.23	9	-5.7	-5.6	-6.5	0.00%	0.00%	0.00%
Cyproconazole		94361-06-5	94361065	1022	Pest_266	6147	4.10	0.69	28	1.92	0.89		-5.0	-5.6	-6.4	0.00%	0.00%	0.00%
Triticonazole		131983-72-7	131983727	424	Pest_57	6148	3.58	0.69	24	1.96	1.44		-4.9	-5.6	-6.2	0.00%	0.00%	0.00%
Fomesafen		72178-02-0	72178020	824	Pest_226	6149	5.40	1.01	8	4.09	1.08		-5.0	-5.6	-6.5	0.00%	0.00%	0.00%
Chlorbromuron		13360-45-7	13360457	428	Pest_60	6150	3.60	1.02	36	2.60	1.02		-5.6	-5.6	-6.3	0.00%	0.00%	0.00%
Imazalil		35554-44-0	35554440	614	Pest_162	6151	3.35	0.69	20	3.21	0.92		-5.7	-5.6	-6.3	0.00%	0.00%	0.00%
Metolachlor		51218-45-2	51218452	56	Pest_180	6152	3.83	0.82	33	2.15	1.28	17	-5.7	-5.6	-6.3	0.00%	0.00%	0.00%
Dimefuron		34205-21-5	34205215	4905	Pest_328	6153	2.48	1.51	3				-5.2	-5.7	-7.3	0.00%	0.00%	0.00%
Propoxur		114-26-1	114261	337	Pest_26	6154	2.88	1.08	53	2.20	0.97	5	-5.8	-5.7	-6.4	0.00%	0.00%	0.00%
Bupirimate		41483-43-6	41483436	633	Pest_174	6155	3.35	0.83	3	2.35	0.83		-5.4	-5.7	-6.8	0.00%	0.00%	0.00%
Metosulam		139528-85-1	139528851	1922	Pest_70	6156	4.15	1.80	3	3.15	1.80		-5.1	-5.7	-7.1	0.00%	0.00%	0.00%
Methidathion		950-37-8	950378	1025	Pest_268	6157	2.68	1.54	26	-0.59	1.01	4	-5.7	-5.7	-6.6	0.00%	0.00%	0.00%
Formothion		2540-82-1	2540821	569	Pest_134	6158	4.46	1.38	21	3.46	1.38		-5.3	-5.7	-6.9	0.00%	0.00%	0.00%
Hymexazol		10004-44-1	10004441	121	Pest_1	6159	4.75	0.88	11	3.41	1.62	4	-5.7	-5.7	-7.3	0.00%	0.00%	0.00%
Carbofuran		1563-66-2	1563662	491	Pest_84	6160	2.46	0.99	61	1.55	1.08	12	-5.6	-5.7	-6.5	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Metconazole		125116-23-6	125116236	405	Pest_48	6161	3.52	0.69	4	2.41	0.69		-5.8	-5.7	-6.3	0.00%	0.00%	0.00%
Azinphos-methyl		86-50-0	86500	972	Pest_258	6162	1.50	1.30	74	0.16	1.05	17	-5.3	-5.7	-6.5	0.00%	0.00%	0.00%
Fenbuconazole		114369-43-6	114369436	338	Pest_27	6163	2.89	0.69	48	2.05	0.62		-5.2	-5.7	-6.3	0.00%	0.00%	0.00%
Dinitramine		29091-05-2	29091052	4910	Pest_331	6164	3.11	0.26	10	2.11	0.26		-5.8	-5.7	-7.1	0.00%	0.00%	0.00%
Triazoxide		72459-58-6	72459586	5175	Pest_429	6165							-5.4	-5.7	-7.4	0.00%	0.00%	0.00%
Ethiofencarb		29973-13-5	29973135	593	Pest_144	6166	3.91	0.93	5	2.91	1.10		-5.9	-5.7	-6.7	0.00%	0.00%	0.00%
Fenamiphos		22224-92-6	22224926	540	Pest_118	6167	1.73	0.97	13	0.73	0.97	13	-5.9	-5.7	-6.8	0.00%	0.00%	0.00%
Diflufenican		83164-33-4	83164334	951	Pest_250	6168	3.18	1.90	6	2.22	1.23		-5.2	-5.8	-6.3	0.00%	0.00%	0.00%
Flupoxam		119126-15-7	119126157	1684	Pest_33	6169	3.38		2				-5.1	-5.8	-6.9	0.00%	0.00%	0.00%
Thiofanox		39196-18-4	39196184	623	Pest_167	6170	2.32		2				-5.9	-5.8	-6.6	0.00%	0.00%	0.00%
Butocarboxim		34681-10-2	34681102	610	Pest_160	6171	4.42	0.60	4	3.42	0.85		-5.9	-5.8	-6.7	0.00%	0.00%	0.00%
Terbacil		5902-51-2	5902512	5149	Pest_424	6172	4.84	0.45	10	1.73	1.05		-5.4	-5.8	-7.4	0.00%	0.00%	0.00%
Anilazine		101-05-3	101053	141	Pest_2	6173	2.43	0.61	17	1.94	0.84	3	-5.9	-5.8	-6.5	0.00%	0.00%	0.00%
Tebufenozide		112410-23-8	112410238	328	Pest_23	6174	3.12	0.63	16	2.08	0.62	7	-5.8	-5.8	-7.2	0.00%	0.00%	0.00%
Dichlorprop-P		15165-67-0	15165670	4896	Pest_323	6175	5.42	0.76	7	4.42	0.76		-5.5	-5.8	-7.2	0.00%	0.00%	0.00%
Mefenacet		73250-68-7	73250687	830	Pest_231	6176	2.75		2				-5.1	-5.8	-6.5	0.00%	0.00%	0.00%
Naptalam		132-66-1	132661	5059	Pest_381	6177	5.14	0.63	9	4.14	0.63		-5.2	-5.8	-7.2	0.00%	0.00%	0.00%
Ofurace		58810-48-3	58810483	5077	Pest_384	6178	2.86	0.47	3				-5.5	-5.8	-7.5	0.00%	0.00%	0.00%
Oxadixyl		77732-09-3	77732093	5080	Pest_388	6179	5.43	0.32	6	4.43	0.32		-5.4	-5.8	-7.4	0.00%	0.00%	0.00%
Metalaxyl-M		70630-17-0	70630170	1113	Pest_375	6180	4.74	0.46	5	3.87	0.49		-5.4	-5.8	-7.1	0.00%	0.00%	0.00%
Propiconazole		60207-90-1	60207901	748	Pest_203	6181	3.43	0.76	38	2.41	1.16	16	-5.9	-5.8	-6.3	0.00%	0.00%	0.00%
Formetanate		22259-30-9	22259309	4963	Pest_357	6182	1.89		1				-5.6	-5.8	-7.8	0.00%	0.00%	0.00%
Desmedipham		13684-56-5	13684565	439	Pest_65	6183	3.18	0.40	6	1.86	0.41		-5.6	-5.9	-6.5	0.00%	0.00%	0.00%
Bendiocarb		22781-23-3	22781233	544	Pest_120	6184	2.29	0.75	18	1.52	1.07	18	-5.6	-5.9	-6.8	0.00%	0.00%	0.00%
Ethirimol		23947-60-6	23947606	555	Pest_127	6185	4.99	0.59	3	3.99	0.59		-5.6	-5.9	-6.6	0.00%	0.00%	0.00%
2,4-DB		94-82-6	94826	4327	Pest_279	6186	4.20	0.35	6	3.20	0.35		-6.0	-5.9	-7.3	0.00%	0.00%	0.00%
Dicofol		115-32-2	115322	340	Pest_28	6187	2.65	0.61	29	1.17	0.46	3	-6.0	-5.9	-6.5	0.00%	0.00%	0.00%
Pymetrozine		123312-89-0	123312890	387	Pest_46	6188	4.80	0.59	7	3.54	1.39		-5.9	-5.9	-7.3	0.00%	0.00%	0.00%
Dichlorprop		120-36-5	120365	4895	Pest_322	6189	3.91	1.08	11	3.86	1.42	3	-5.6	-5.9	-7.3	0.00%	0.00%	0.00%
Phosmet		732-11-6	732116	828	Pest_230	6190	2.67	1.35	33	0.10	0.51	4	-5.4	-5.9	-7.3	0.00%	0.00%	0.00%
Quintozene		82-68-8	82688	5115	Pest_407	6191	2.30	0.77	8	1.51	0.41		-6.0	-5.9	-6.5	0.00%	0.00%	0.00%
Quinalphos		13593-03-8	13593038	437	Pest_63	6192	2.55	1.21	15	1.55	1.38	45	-6.0	-5.9	-6.6	0.00%	0.00%	0.00%
Oxydemeton-methyl		301-12-2	301122	595	Pest_146	6193	3.26	1.00	17	2.26	1.13	17	-5.3	-5.9	-6.6	0.00%	0.00%	0.00%
Ethephon		16672-87-0	16672870	505	Pest_89	6194	5.27	0.33	10	4.27	0.33		-5.6	-5.9	-6.8	0.00%	0.00%	0.00%
Triclopyr		55335-06-3	55335063	698	Pest_191	6195	3.56	0.89	14	3.31	0.64	4	-5.4	-5.9	-6.6	0.00%	0.00%	0.00%
Dimoxystrobin		149961-52-4	149961524	481	Pest_78	6196	1.54	0.21	4	0.93	0.56		-5.2	-5.9	-6.9	0.00%	0.00%	0.00%
Butralin		33629-47-9	33629479	605	Pest_154	6197	2.30	0.91	21	0.48	0.34		-5.9	-5.9	-6.4	0.00%	0.00%	0.00%
Quinclorac		84087-01-4	84087014	958	Pest_253	6198	4.60	0.49	13	3.01	0.86	11	-5.4	-5.9	-7.0	0.00%	0.00%	0.00%
Trietazine		1912-26-1	1912261	518	Pest_105	6199	3.78		1				-6.1	-6.0	-6.6	0.00%	0.00%	0.00%
Propamocarb		24579-73-5	24579735	5105	Pest_400	6200	5.24	1.07	36	4.43	0.45		-6.1	-6.0	-7.8	0.00%	0.00%	0.00%
MCPB		94-81-5	94815	5015	Pest_370	6201	3.15	1.17	3	2.15	1.17		-5.9	-6.0	-7.3	0.00%	0.00%	0.00%
Bromoxynil		1689-84-5	1689845	34	Pest_92	6202	3.47	0.87	15	2.76	1.27	3	-5.4	-6.0	-6.5	0.00%	0.00%	0.00%
Picoxystrobine		117428-22-5	117428225	5095	Pest_396	6203	1.84	0.42	3				-5.9	-6.0	-7.4	0.00%	0.00%	0.00%
Difenoconazole		119446-68-3	119446683	351	Pest_35	6204	2.67	0.69	48	0.32	0.84		-5.5	-6.0	-6.4	0.00%	0.00%	0.00%
Metalaxyl		57837-19-1	57837191	726	Pest_199	6205	4.93	0.80	21	4.51	0.59	5	-5.6	-6.0	-7.2	0.00%	0.00%	0.00%
Iprovalicarb		140923-17-7	140923177	453	Pest_71	6206	4.49	1.07	6	3.49	1.07		-5.4	-6.0	-6.9	0.00%	0.00%	0.00%
Furalaxyl		57646-30-7	57646307	725	Pest_198	6207	4.57	0.36	6	3.57	0.36		-5.7	-6.0	-7.3	0.00%	0.00%	0.00%
Triazophos		24017-47-8	24017478	557	Pest_129	6208	2.66	1.63	6	0.37	0.80		-6.1	-6.0	-6.7	0.00%	0.00%	0.00%
Fenitrothion		122-14-5	122145	378	Pest_42	6209	2.20	1.40	138	1.88	0.97	18	-6.1	-6.0	-6.7	0.00%	0.00%	0.00%
Pyraclostrobin		175013-18-0	175013180	512	Pest_97	6210	1.32	0.73	8	1.17	1.00		-5.2	-6.0	-6.8	0.00%	0.00%	0.00%
Pirimiphos-Methyl		29232-93-7	29232937	586	Pest_141	6211	1.90	1.47	25	1.78	1.38	18	-6.1	-6.0	-6.7	0.00%	0.00%	0.00%
prothiocarb		19622-08-3	19622083	5109	Pest_403	6212	3.93	0.83	3				-5.7	-6.0	-7.8	0.00%	0.00%	0.00%
Cycluron		2163-69-1	2163691	4880	Pest_315	6213	3.69	0.94	3				-5.9	-6.0	-7.4	0.00%	0.00%	0.00%
Ioxynil		1689-83-4	1689834	507	Pest_91	6214	3.80	0.18	8	2.80	0.18		-5.1	-6.0	-6.5	0.00%	0.00%	0.00%
Tetradifon		116-29-0	116290	344	Pest_31	6215	3.17	0.81	8	2.17	0.55		-6.2	-6.1	-6.8	0.00%	0.00%	0.00%
Bromopropylate		18181-80-1	18181801	4865	Pest_295	6216	3.16	0.60	9	2.16	0.55		-6.1	-6.1	-7.5	0.00%	0.00%	0.00%
Chlorfenapyr		122453-73-0	122453730	380	Pest_44	6217	1.17	0.82	7	0.17	0.82		-6.1	-6.1	-7.5	0.00%	0.00%	0.00%
Benzoximate		29104-30-1	29104301	4847	Pest_291	6218							-6.1	-6.1	-7.5	0.00%	0.00%	0.00%
Fenazaquin		120928-09-8	120928098	366	Pest_39	6219	1.51	1.11	12	0.22	0.42	3	-6.1	-6.1	-7.5	0.00%	0.00%	0.00%
Fluoroglycofen		77501-60-1	77501601	4959	Pest_354	6220	3.40	0.97	3				-5.4	-6.1	-7.5	0.00%	0.00%	0.00%
Haloxyfop		69806-34-4	69806344	810	Pest_222	6221	5.50	0.84	28	4.36	0.84		-5.7	-6.1	-6.5	0.00%	0.00%	0.00%
Prohexadione-calcium		127277-53-6	127277536	6311	Pest_399	6222	4.63	0.77	9	3.31	0.62		-6.1	-6.1	-7.5	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Sodium paranitrophenolate		824-78-2	824782	6327	Pest_414	6223							-6.1	-6.1	-7.5	0.00%	0.00%	0.00%
Sodium 5-nitroguaiacolate		67233-85-6	67233856	6324	Pest_412	6224							-6.1	-6.1	-7.5	0.00%	0.00%	0.00%
Sodium orthonitrophenolate		824-39-5	824395	6326	Pest_413	6225							-6.1	-6.1	-7.5	0.00%	0.00%	0.00%
Pyrimethanil		53112-28-0	53112280	681	Pest_186	6226	3.78	0.83	15	1.97	0.79		-6.0	-6.1	-6.7	0.00%	0.00%	0.00%
Penconazole		66246-88-6	66246886	787	Pest_213	6227	3.60	0.69	24	2.60	0.69		-6.2	-6.1	-6.9	0.00%	0.00%	0.00%
Chlorfenvinphos		470-90-6	470906	1098	Pest_301	6228	2.12	1.52	26	1.12	1.01	78	-6.2	-6.1	-6.7	0.00%	0.00%	0.00%
Phoxim		14816-18-3	14816183	475	Pest_76	6229	2.30	0.95	17	2.02	0.13	6	-6.2	-6.1	-6.9	0.00%	0.00%	0.00%
Benazolin		3813-05-6	3813056	116	Pest_165	6230	5.10	0.57	4	4.10	0.81		-5.6	-6.1	-6.9	0.00%	0.00%	0.00%
Fenoxaprop-P		113158-40-0	113158400	335	Pest_25	6231	2.29	1.48	6	0.89	0.84		-5.3	-6.1	-6.6	0.00%	0.00%	0.00%
Cymoxanil		57966-95-7	57966957	727	Pest_200	6232	4.11	0.80	16	2.47	0.90	9	-5.3	-6.1	-7.3	0.00%	0.00%	0.00%
Chlorpyrifos		2921-88-2	2921882	585	Pest_140	6233	1.05	1.40	195	0.36	1.46	83	-6.3	-6.1	-6.6	0.00%	0.00%	0.00%
Fenpropimorph		67564-91-4	67564914	4949	Pest_344	6234	3.28	0.71	10	1.23	1.51		-6.2	-6.1	-7.3	0.00%	0.00%	0.00%
Parathion		56-38-2	56382	713	Pest_196	6235	1.67	1.49	119	-0.30	1.27	12	-6.2	-6.1	-6.7	0.00%	0.00%	0.00%
Fluazifop		69335-91-7	69335917	1112	Pest_350	6236	3.74	0.54	3				-5.5	-6.1	-6.6	0.00%	0.00%	0.00%
Isoxaben		82558-50-7	82558507	946	Pest_246	6237	3.17	0.65	12	3.02	0.43	7	-5.4	-6.2	-7.2	0.00%	0.00%	0.00%
Azinphos-ethyl		2642-71-9	2642719	40	Pest_137	6238	1.31	1.28	8	0.31	1.38		-5.6	-6.2	-6.7	0.00%	0.00%	0.00%
Maleic hydrazide		123-33-1	123331	389	Pest_47	6239	5.18	0.66	5	4.49	0.43		-5.7	-6.2	-7.0	0.00%	0.00%	0.00%
Clodinafop		114420-56-3	114420563	4877	Pest_304	6240	3.35	1.15	3				-5.7	-6.2	-7.9	0.00%	0.00%	0.00%
Ethalfluralin		55283-68-6	55283686	695	Pest_189	6241	2.12	0.91	24	0.92	0.70		-6.3	-6.2	-6.7	0.00%	0.00%	0.00%
Tolclofos-methyl		57018-04-9	57018049	718	Pest_197	6242	3.48	1.01	15	2.48	1.01		-6.3	-6.2	-6.7	0.00%	0.00%	0.00%
Isopropalin		33820-53-0	33820530	4982	Pest_365	6243	2.96	1.01	4	1.04	0.64		-5.8	-6.2	-7.1	0.00%	0.00%	0.00%
Acifluorfen		50594-66-6	50594666	4828	Pest_283	6244	3.01	1.01	5	2.01	1.01		-5.9	-6.2	-7.5	0.00%	0.00%	0.00%
EPTC		759-94-4	759944	869	Reach_1529	6245	3.96	0.46	29	3.33	0.72	8	-6.3	-6.2	-7.1	0.00%	0.00%	0.00%
Malathion		121-75-5	121755	374	Pest_41	6246	2.45	1.32	208	1.66	1.45	39	-6.3	-6.2	-7.2	0.00%	0.00%	0.00%
Flusilazole		85509-19-9	85509199	967	Pest_256	6247	3.75	0.69	8	2.75	0.69		-6.3	-6.2	-6.7	0.00%	0.00%	0.00%
Phosalone		2310-17-0	2310170	546	Pest_122	6248	2.54	1.11	19	1.54	1.38	57	-6.2	-6.3	-6.8	0.00%	0.00%	0.00%
Diazinon		333-41-5	333415	47	Pest_152	6249	2.34	1.65	95	0.80	1.77	28	-6.4	-6.3	-6.8	0.00%	0.00%	0.00%
Zoxamide		156052-68-5	156052685	490	Pest_83	6250	2.56	0.61	12	1.16	1.45	7	-5.7	-6.3	-7.2	0.00%	0.00%	0.00%
Dichlofluanid		1085-98-9	1085989	241	Pest_17	6251	2.71	1.07	11	1.71	1.07	11	-6.4	-6.3	-7.1	0.00%	0.00%	0.00%
Thiobencarb		28249-77-6	28249776	580	Pest_138	6252	3.08	0.58	49	1.63	0.91	16	-6.4	-6.3	-7.3	0.00%	0.00%	0.00%
Prochloraz		67747-09-5	67747095	797	Pest_217	6253	3.28	0.50	8	2.00	0.47		-5.7	-6.3	-7.3	0.00%	0.00%	0.00%
Propaquizafop		111479-05-1	111479051	303	Pest_19	6254	2.90	0.84	20	1.90	0.84		-5.6	-6.3	-7.2	0.00%	0.00%	0.00%
Parathion-Methyl		298-00-0	298000	5086	Pest_392	6255	2.95	1.40	112	2.06	1.46	11	-6.5	-6.3	-7.9	0.00%	0.00%	0.00%
Kresoxim-Methyl		143390-89-0	143390890	470	Pest_74	6256	2.20	0.46	11	2.07	0.57	8	-6.1	-6.3	-7.3	0.00%	0.00%	0.00%
Benfuracarb		82560-54-1	82560541	947	Pest_247	6257	2.55	1.39	5	1.55	1.39		-6.3	-6.3	-7.0	0.00%	0.00%	0.00%
Mevinphos		7786-34-7	7786347	5035	Pest_378	6258	1.71	1.04	33	0.68	1.01	15	-6.4	-6.3	-8.3	0.00%	0.00%	0.00%
Bromacil		314-40-9	314409	4864	Pest_294	6259	4.70	0.73	13	1.48	1.25	10	-5.8	-6.3	-8.0	0.00%	0.00%	0.00%
Cyprodinil		121552-61-2	121552612	371	Pest_40	6260	3.02	0.71	18	2.12	1.04	8	-6.4	-6.3	-6.8	0.00%	0.00%	0.00%
Thiamethoxam		153719-23-4	153719234	487	Pest_81	6261	3.61	1.51	15	3.40	1.53	3	-6.1	-6.3	-7.2	0.00%	0.00%	0.00%
Desmetryn		1014-69-3	1014693	149	Pest_8	6262	3.83	1.00	7	2.83	1.09		-6.5	-6.3	-7.1	0.00%	0.00%	0.00%
Guazatine		13516-27-3	13516273	4970	Pest_360	6263	3.03	1.10	3				-5.7	-6.3	-8.0	0.00%	0.00%	0.00%
Fenoxycarb		72490-01-8	72490018	825	Pest_227	6264	3.06	0.35	11	2.06	0.35	11	-6.3	-6.4	-6.9	0.00%	0.00%	0.00%
Monalide		7287-36-7	7287367	5040	Pest_379	6265	2.68	0.44	3				-6.5	-6.4	-7.7	0.00%	0.00%	0.00%
Tebutam		35256-85-0	35256850	5143	Pest_420	6266	3.11	0.64	3				-6.5	-6.4	-7.3	0.00%	0.00%	0.00%
Thidiazuron		51707-55-2	51707552	5158	Pest_426	6267	3.84	1.02	27	2.57	0.79		-5.8	-6.4	-7.9	0.00%	0.00%	0.00%
Fluorodifen		15457-05-3	15457053	4958	Pest_353	6268	4.36	1.01	4	3.36	1.01		-6.5	-6.4	-7.9	0.00%	0.00%	0.00%
Tetraconazole		112281-77-3	112281773	323	Pest_22	6269	3.40	0.69	40	2.36	0.69		-6.5	-6.4	-7.0	0.00%	0.00%	0.00%
Endosulfan		115-29-7	115297	4921	Pest_337	6270	0.96	1.24	130	0.59	1.00	15	-6.5	-6.4	-7.2	0.00%	0.00%	0.00%
Neburon		555-37-3	555373	5063	Pest_382	6271	2.94	1.02	6	1.94	1.02		-6.4	-6.4	-7.5	0.00%	0.00%	0.00%
Propham		122-42-9	122429	5107	Pest_401	6272	4.16	0.49	13	3.16	0.49	13	-6.6	-6.4	-7.7	0.00%	0.00%	0.00%
Thiometon		640-15-3	640153	775	Pest_208	6273	3.86	1.38	39	2.86	1.38		-6.6	-6.4	-6.9	0.00%	0.00%	0.00%
Quizalofop		76578-12-6	76578126	5116	Pest_408	6274	4.69	0.84	8	4.18	0.84		-5.7	-6.5	-7.9	0.00%	0.00%	0.00%
Mepiquat		15302-91-7	15302917	5017	Pest_372	6275	5.27	0.96	3				-6.2	-6.5	-8.5	0.00%	0.00%	0.00%
Phosthiazate		98886-44-3	98886443	5094	Pest_395	6276	4.02	1.21	6	3.04	0.90		-6.3	-6.5	-7.9	0.00%	0.00%	0.00%
Methoprotryne		841-06-5	841065	959	Pest_254	6277	4.27	1.09	7	3.27	1.09		-6.1	-6.5	-7.5	0.00%	0.00%	0.00%
Benfluralin		1861-40-1	1861401	514	Pest_99	6278	3.16	1.00	14	1.18	0.91	18	-6.6	-6.5	-6.9	0.00%	0.00%	0.00%
Bifenox		42576-02-3	42576023	4851	Pest_293	6279	3.36	1.23	9	2.36	1.01		-6.6	-6.5	-8.0	0.00%	0.00%	0.00%
Fonofos		944-22-9	944229	1023	Pest_267	6280	1.85	1.09	16	0.10	0.89	8	-6.6	-6.5	-7.0	0.00%	0.00%	0.00%
Diflubenzuron		35367-38-5	35367385	612	Pest_161	6281	2.41	2.45	40	1.39	2.04	24	-5.9	-6.5	-7.3	0.00%	0.00%	0.00%
Chlozolinate		84332-86-5	84332865	3860	Pest_255	6282	3.57	0.65	3				-6.0	-6.5	-8.2	0.00%	0.00%	0.00%
Trifloxystrobine		141517-21-7	141517217	5178	Pest_431	6283	1.80	0.67	12	1.71	1.41	4	-6.2	-6.5	-7.4	0.00%	0.00%	0.00%
Difenoxuron		14214-32-5	14214325	4902	Pest_325	6284	3.66	1.28	5	2.66	1.02		-5.8	-6.5	-7.9	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Nitrothal-isopropyl		10552-74-6	10552746	176	Pest_14	6285	3.20	0.84	9	2.20	0.84		-6.6	-6.5	-7.7	0.00%	0.00%	0.00%
Clomazone		81777-89-1	81777891	941	Pest_244	6286	3.91	0.67	9	2.99	0.71		-6.6	-6.5	-7.1	0.00%	0.00%	0.00%
Foramsulfuron		173159-57-4	173159574	510	Pest_95	6287	4.41	1.83	12	4.71	0.56	3	-6.1	-6.5	-7.7	0.00%	0.00%	0.00%
Isofenphos		25311-71-1	25311711	567	Pest_133	6288	2.30	1.38	11	1.44	1.36	3	-6.6	-6.5	-7.5	0.00%	0.00%	0.00%
Pyridate		55512-33-9	55512339	701	Pest_193	6289	3.77	1.03	9	2.77	1.03		-6.2	-6.5	-7.0	0.00%	0.00%	0.00%
Cyclanilide		113136-77-9	113136779	334	Pest_24	6290	4.12	0.32	7	2.06	1.33		-6.1	-6.5	-7.3	0.00%	0.00%	0.00%
Molinate		2212-67-1	2212671	537	Pest_117	6291	3.85	0.67	40	2.72	0.57	14	-6.6	-6.5	-7.0	0.00%	0.00%	0.00%
Trinexapac-Ethyl		95266-40-3	95266403	1026	Pest_269	6292	4.64	0.92	30	2.92	0.92		-6.1	-6.5	-7.7	0.00%	0.00%	0.00%
Cypromazine		66215-27-8	66215278	4881	Pest_318	6293	5.03	1.70	30	4.17	1.25		-6.1	-6.5	-7.9	0.00%	0.00%	0.00%
Amitraz		33089-61-1	33089611	603	Pest_151	6294	3.41	0.98	13	2.41	0.98	13	-6.5	-6.5	-7.1	0.00%	0.00%	0.00%
Fenthion		55-38-9	55389	699	Pest_192	6295	1.82	1.35	114	1.55	1.81	12	-6.6	-6.5	-7.0	0.00%	0.00%	0.00%
Ametryn		834-12-8	834128	953	Reach_1562	6296	3.09	1.19	35	1.56	1.27	7	-6.6	-6.5	-7.2	0.00%	0.00%	0.00%
Fenothiocarb		62850-32-2	62850322	4946	Pest_341	6297	3.86	0.61	6	2.86	0.61		-6.7	-6.5	-8.0	0.00%	0.00%	0.00%
Fenamidone		161326-34-7	161326347	499	Pest_87	6298	2.54	0.66	6	1.96	0.75		-5.8	-6.6	-7.0	0.00%	0.00%	0.00%
Amidosulfuron		120923-37-7	120923377	365	Pest_38	6299	4.18	2.39	3	0.88			-6.1	-6.6	-7.7	0.00%	0.00%	0.00%
Nicosulfuron		111991-09-4	111991094	319	Pest_21	6300	4.90	1.34	5	4.61	1.32		-6.2	-6.6	-8.0	0.00%	0.00%	0.00%
Chlorpyrifos-Methyl		5598-13-0	5598130	709	Pest_194	6301	1.42	1.59	22	0.42	1.38	66	-6.7	-6.6	-7.0	0.00%	0.00%	0.00%
Etridiazole		2593-15-9	2593159	571	Pest_135	6302	3.47	0.43	11	1.74	1.05	8	-6.9	-6.6	-8.3	0.00%	0.00%	0.00%
Fenoxaprop		95617-09-7	95617097	4947	Pest_342	6303	3.12	0.66	4	2.12	0.66		-5.8	-6.6	-7.9	0.00%	0.00%	0.00%
Terbutryn		886-50-0	886500	104	Pest_260	6304	2.47	1.12	35	1.19	1.09	22	-6.7	-6.6	-7.2	0.00%	0.00%	0.00%
Sulfosulfuron		141776-32-1	141776321	457	Pest_72	6305	5.01	1.32	12	3.43	1.96		-6.2	-6.6	-7.5	0.00%	0.00%	0.00%
Sulfotep		3689-24-5	3689245	5137	Pest_417	6306	1.40	1.09	7	0.40	1.38		-6.7	-6.6	-7.5	0.00%	0.00%	0.00%
Prosulfuron		94125-34-5	94125345	1021	Pest_265	6307	2.94	1.32	18	1.94	2.04		-6.6	-6.6	-8.0	0.00%	0.00%	0.00%
Carboxin		5234-68-4	5234684	673	Pest_181	6308	4.05	0.81	9	2.40	0.41		-6.1	-6.6	-8.0	0.00%	0.00%	0.00%
Quizalofop-P-ethyl		100646-51-3	100646513	5117	Pest_409	6309	3.36	1.20	8	2.04	0.99		-6.4	-6.6	-7.9	0.00%	0.00%	0.00%
Vernolate		1929-77-7	1929777	521	Pest_108	6310	3.40	0.55	16	2.77	0.71	3	-6.8	-6.6	-7.5	0.00%	0.00%	0.00%
Flazasulfuron		104040-78-0	104040780	166	Pest_12	6311	3.91	1.98	11	3.37	1.24	3	-6.3	-6.6	-7.6	0.00%	0.00%	0.00%
Benalaxyl		71626-11-4	71626114	823	Pest_225	6312	4.04	0.33	8	2.65	0.50		-6.5	-6.6	-7.6	0.00%	0.00%	0.00%
Profenofos		41198-08-7	41198087	631	Reach_2738	6313	1.55	1.09	37	1.11	1.66	13	-6.7	-6.6	-7.1	0.00%	0.00%	0.00%
Rimsulfuron		122931-48-0	122931480	383	Pest_45	6314	5.18	1.32	20	1.01	1.10		-6.2	-6.6	-7.6	0.00%	0.00%	0.00%
Dialifos		10311-84-9	10311849	4894	Pest_321	6315	1.04	1.38	6	0.19	1.38		-6.1	-6.6	-8.0	0.00%	0.00%	0.00%
Cycloxydim		101205-02-1	101205021	144	Pest_4	6316	5.03	0.76	4	4.03	0.76		-5.7	-6.6	-7.3	0.00%	0.00%	0.00%
Chlormephos		24934-91-6	24934916	564	Pest_132	6317	2.68	0.85	3	1.68	1.13		-6.8	-6.6	-7.1	0.00%	0.00%	0.00%
Cyanamide		420-04-2	420042	636	Reach_1268	6318	3.96	0.73	12	2.99	0.86	5	-6.8	-6.6	-7.5	0.00%	0.00%	0.00%
Disulfoton		298-04-4	298044	590	Pest_143	6319	2.58	1.18	27	1.42	1.26	6	-6.8	-6.6	-7.1	0.00%	0.00%	0.00%
Fenhexamid		126833-17-8	126833178	409	Pest_50	6320	3.57	0.67	8	2.94	0.66		-5.9	-6.7	-7.2	0.00%	0.00%	0.00%
Cycloate		1134-23-2	1134232	4878	Pest_314	6321	3.78	0.61	21	2.78	0.61		-6.8	-6.7	-7.9	0.00%	0.00%	0.00%
Mepronil		55814-41-0	55814410	5018	Pest_373	6322	4.00		1				-6.5	-6.7	-8.0	0.00%	0.00%	0.00%
Ethoprophos		13194-48-4	13194484	4930	Pest_339	6323	2.58	1.22	21	1.08	0.90	6	-6.8	-6.7	-7.9	0.00%	0.00%	0.00%
Ethion		563-12-2	563122	711	Pest_195	6324	1.96	1.31	27	1.67	1.38	12	-6.7	-6.7	-7.2	0.00%	0.00%	0.00%
Phorate		298-02-2	298022	589	Pest_142	6325	1.19	1.15	30	-0.60	0.83	5	-6.8	-6.7	-7.2	0.00%	0.00%	0.00%
Chlorpropham		101-21-3	101213	145	Pest_5	6326	3.68	0.17	7	2.68	0.17		-6.8	-6.7	-7.2	0.00%	0.00%	0.00%
Chlorfenson		80-33-1	80331	935	Pest_243	6327	4.30	0.55	6	3.30	0.55		-6.8	-6.7	-7.4	0.00%	0.00%	0.00%
Oxyfluorfen		42874-03-3	42874033	638	Pest_175	6328	2.48	1.51	13	1.42	0.68	8	-6.8	-6.7	-7.2	0.00%	0.00%	0.00%
Carbosulfan		55285-14-8	55285148	696	Pest_190	6329	2.08	1.42	10	1.04	0.61		-6.3	-6.7	-7.1	0.00%	0.00%	0.00%
Tralkoxydim		87820-88-0	87820880	981	Pest_259	6330	4.03	0.65	5	3.85	0.66		-5.9	-6.7	-7.5	0.00%	0.00%	0.00%
Oxadiargyl		39807-15-3	39807153	626	Pest_169	6331	4.63	0.81	4	3.63	0.81		-6.4	-6.7	-7.3	0.00%	0.00%	0.00%
Quinoclamine		2797-51-5	2797515	5113	Pest_405	6332	3.40	0.14	4	2.40	0.14		-6.5	-6.8	-8.4	0.00%	0.00%	0.00%
Lindane		58-89-9	58899	68	Pest_367	6333	2.07	1.05	157	1.68	1.28	21	-6.9	-6.8	-7.5	0.00%	0.00%	0.00%
Quinomethionate		2439-01-2	2439012	5114	Pest_406	6334	2.65	1.38	12	0.90	0.46	5	-6.6	-6.8	-8.2	0.00%	0.00%	0.00%
Acidenzolar		126448-41-7	126448417	4827	Pest_282	6335	3.49	0.60	3				-6.4	-6.8	-8.6	0.00%	0.00%	0.00%
Furathiocarb		65907-30-4	65907304	3457	Pest_211	6336	2.50	1.48	3				-6.5	-6.8	-8.1	0.00%	0.00%	0.00%
Flurochloridone		61213-25-0	61213250	4960	Pest_355	6337	3.63	0.81	16	2.63	0.81		-6.9	-6.8	-8.1	0.00%	0.00%	0.00%
Tri-allate		2303-17-5	2303175	545	Pest_121	6338	2.81	0.65	17	1.78	0.61	18	-6.9	-6.8	-7.6	0.00%	0.00%	0.00%
carbophenothion		786-19-6	786196	898	Pest_237	6339	1.56	1.19	29	0.32	0.49	4	-6.8	-6.8	-7.3	0.00%	0.00%	0.00%
Cadusafos		95465-99-9	95465999	1027	Pest_270	6340	2.66	1.36	8	1.66	1.13		-7.0	-6.8	-7.3	0.00%	0.00%	0.00%
Aldimorph		91315-15-0	91315150	4833	Pest_285	6341	2.14	0.36	3				-7.0	-6.8	-8.1	0.00%	0.00%	0.00%
Dinoterb		1420-07-1	1420071	4911	Pest_333	6342	2.01	1.29	5	1.01	0.71		-6.4	-6.8	-8.5	0.00%	0.00%	0.00%
Fluazifop-P-butyl		79241-46-6	79241466	4954	Pest_351	6343	3.27	1.18	10	2.27	1.18		-6.9	-6.8	-8.0	0.00%	0.00%	0.00%
Sethoxydim		74051-80-2	74051802	834	Pest_232	6344	4.01	0.97	16	3.46	0.93	8	-6.0	-6.9	-7.5	0.00%	0.00%	0.00%
Clethodim		99129-21-2	99129212	1084	Pest_275	6345	4.69	0.76	8	3.72	1.02		-5.9	-6.9	-7.4	0.00%	0.00%	0.00%
Flurtamone		96525-23-4	96525234	4150	Pest_272	6346	2.66	1.50	3				-6.4	-6.9	-8.5	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [-]	Z(Cwfresh) [-]	Z(Cwcoast) [-]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Tridemorph		24602-86-6	24602866	2398	Pest_130	6347	1.93	0.30	3				-7.1	-6.9	-8.8	0.00%	0.00%	0.00%
Azocyclotin		41083-11-8	41083118	630	Pest_171	6348	1.04	1.06	12	0.04	1.06		-6.2	-6.9	-7.2	0.00%	0.00%	0.00%
Triflumuron		64628-44-0	64628440	3441	Pest_209	6349	1.78	1.41	3				-6.3	-6.9	-8.2	0.00%	0.00%	0.00%
Fenpiclonil		74738-17-3	74738173	4948	Pest_343	6350	2.91	0.29	6	1.91	0.29		-6.9	-6.9	-8.2	0.00%	0.00%	0.00%
Temephos		3383-96-8	3383968	5146	Pest_422	6351	1.75	1.58	101	0.99	1.51	16	-6.7	-6.9	-7.7	0.00%	0.00%	0.00%
Oxadiazon		19666-30-9	19666309	526	Pest_110	6352	3.16	0.81	56	1.21	1.04		-6.8	-6.9	-7.4	0.00%	0.00%	0.00%
Methoxyfenozide		161050-58-4	161050584	5021	Pest_376	6353	3.41	0.25	6	2.33	0.87		-6.4	-7.0	-8.6	0.00%	0.00%	0.00%
Terbufos		13071-79-9	13071799	416	Pest_51	6354	1.10	1.09	24	-0.26	0.95	9	-7.1	-7.0	-7.5	0.00%	0.00%	0.00%
Fipronil		120068-37-3	120068373	11	Pest_37	6355	1.43	1.05	32	0.26	1.05	44	-6.3	-7.0	-7.5	0.00%	0.00%	0.00%
Spiroxamine		118134-30-8	118134308	347	Pest_32	6356	1.87	1.69	7	1.28	1.01		-6.9	-7.0	-7.5	0.00%	0.00%	0.00%
Thifensulfuron-methyl		79277-27-3	79277273	918	Pest_238	6357	5.21	0.95	18	1.64	1.58		-6.5	-7.0	-8.4	0.00%	0.00%	0.00%
Teflubenzuron		83121-18-0	83121180	5144	Pest_421	6358	4.14	2.70	3	3.14	1.70		-6.4	-7.0	-8.2	0.00%	0.00%	0.00%
Flutolanil		66332-96-5	66332965	4961	Pest_356	6359	3.72	0.57	18	3.06	1.03	10	-7.1	-7.0	-8.4	0.00%	0.00%	0.00%
Haloxyfop-R		95977-29-0	95977290	4971	Pest_361	6360	3.38		2				-6.5	-7.1	-8.3	0.00%	0.00%	0.00%
4-CPA		122-88-3	122883	4795	Pest_280	6361	5.26		1				-6.8	-7.1	-8.9	0.00%	0.00%	0.00%
Bensulfuron-methyl		83055-99-6	83055996	949	Pest_249	6362	5.02	0.95	39	3.93	1.07		-6.6	-7.1	-8.6	0.00%	0.00%	0.00%
Tepraloxydim		149979-41-9	149979419	5148	Pest_423	6363	4.32	0.79	5	2.54	0.32		-6.3	-7.1	-8.4	0.00%	0.00%	0.00%
Chlorbufam		1967-16-4	1967164	4870	Pest_300	6364	4.23	0.18	4	3.23	0.18		-7.2	-7.2	-8.1	0.00%	0.00%	0.00%
Metsulfuron-methyl		74223-64-6	74223646	836	Pest_234	6365	3.64	1.82	16	1.52	1.58	9	-6.6	-7.2	-8.4	0.00%	0.00%	0.00%
Hexaflumuron		86479-06-3	86479063	971	Pest_257	6366	1.88	1.48	4	-0.11	1.70		-6.7	-7.2	-7.7	0.00%	0.00%	0.00%
Chlorsulfuron		64902-72-3	64902723	783	Pest_210	6367	3.03	1.81	28	2.49	2.00	15	-6.7	-7.2	-8.1	0.00%	0.00%	0.00%
Paclobutrazol		76738-62-0	76738620	5082	Pest_390	6368	4.35	0.38	11	3.35	0.38	11	-6.6	-7.2	-8.5	0.00%	0.00%	0.00%
Flupyrsulfuron		150315-10-9	150315109	2009	Pest_79	6369	3.81	1.99	3				-6.8	-7.2	-9.2	0.00%	0.00%	0.00%
Cyhexatin		13121-70-5	13121705	419	Pest_52	6370	0.45	1.06	42	-0.70	1.06		-6.5	-7.2	-7.5	0.00%	0.00%	0.00%
Prothiofos		34643-46-4	34643464	2711	Pest_159	6371	1.15	1.10	3				-7.3	-7.3	-8.2	0.00%	0.00%	0.00%
Triasulfuron		82097-50-5	82097505	944	Pest_245	6372	4.49	1.32	18	2.82	2.25		-6.7	-7.3	-8.1	0.00%	0.00%	0.00%
Benfuresate		68505-69-1	68505691	4846	Pest_289	6373	4.06	0.79	3				-7.3	-7.3	-8.8	0.00%	0.00%	0.00%
Mesosulfuron-methyl		208465-21-8	208465218	5020	Pest_374	6374	4.55	0.93	10	3.89	1.19		-6.8	-7.3	-9.2	0.00%	0.00%	0.00%
Fludioxonil		131341-86-1	131341861	420	Pest_53	6375	2.73	0.24	8	1.65	0.72		-6.7	-7.3	-7.8	0.00%	0.00%	0.00%
Azafenidin		68049-83-2	68049832	3505	Pest_218	6376	1.72	2.62	3				-6.5	-7.3	-8.5	0.00%	0.00%	0.00%
Ethoxysulfuron		126801-58-9	126801589	407	Pest_49	6377	3.04		1				-6.8	-7.3	-8.8	0.00%	0.00%	0.00%
Tribenuron-methyl		101200-48-0	101200480	142	Pest_3	6378	4.45	1.95	8	2.13	1.74		-6.7	-7.3	-8.4	0.00%	0.00%	0.00%
Fenpropathrin		39515-41-8	39515418	624	Pest_168	6379	0.69	1.16	17	-1.55	0.65	4	-7.3	-7.5	-7.9	0.00%	0.00%	0.00%
Flufenoxuron		101463-69-8	101463698	148	Pest_7	6380	0.35	1.40	6	-0.84	1.40		-6.6	-7.5	-7.8	0.00%	0.00%	0.00%
Pyridaben		96489-71-3	96489713	1055	Pest_271	6381	0.44	0.57	7	0.33	1.08		-7.2	-7.5	-8.0	0.00%	0.00%	0.00%
Pyridfenox		88283-41-4	88283414	5110	Pest_404	6382	3.46	0.85	5	2.46	0.85		-7.8	-7.5	-9.1	0.00%	0.00%	0.00%
Beta-Cyfluthrin		68359-37-5	68359375	4849	Pest_292	6383	0.30	1.15	21	-1.54	1.05	6	-7.6	-7.5	-8.7	0.00%	0.00%	0.00%
Lufenuron		103055-07-8	103055078	158	Pest_11	6384	3.58	1.70	9	2.58	1.70		-7.1	-7.5	-7.9	0.00%	0.00%	0.00%
Norflurazon		27314-13-2	27314132	5073	Pest_383	6385	3.94	0.20	7	2.11	1.15		-7.2	-7.5	-8.9	0.00%	0.00%	0.00%
Cypermethrin		52315-07-8	52315078	1099	Pest_317	6386	-0.11	1.19	84		1.75	17	-7.1	-7.5	-7.9	0.00%	0.00%	0.00%
Tridiphane		58138-08-2	58138082	5176	Pest_430	6387	2.93	1.43	7	1.93	0.81		-7.6	-7.5	-8.3	0.00%	0.00%	0.00%
Tebufenpyrad		119168-77-3	119168773	350	Pest_34	6388	1.61	0.36	3	0.90	0.28		-7.1	-7.6	-8.1	0.00%	0.00%	0.00%
Triapenthenol		76608-88-3	76608883	5174	Pest_428	6389							-6.9	-7.6	-9.0	0.00%	0.00%	0.00%
Deltamethrin		52918-63-5	52918635	679	Pest_185	6390	0.29	1.59	62	-0.57	1.71	14	-7.1	-7.6	-8.0	0.00%	0.00%	0.00%
Bifenthrin		82657-04-3	82657043	948	Pest_248	6391	0.02	1.26	24	-1.10	1.24	6	-7.3	-7.6	-8.0	0.00%	0.00%	0.00%
Alpha-cypermethrin		67375-30-8	67375308	1108	Pest_287	6392	0.32	0.98	9	-0.68	1.35		-7.2	-7.6	-8.0	0.00%	0.00%	0.00%
Fenpropidin		67306-00-7	67306007	792	Pest_216	6393	1.84	1.81	10	2.67	0.29		-7.9	-7.7	-8.8	0.00%	0.00%	0.00%
Permethrin		52645-53-1	52645531	676	Pest_182	6394	1.08	1.26	104	-0.30	1.70	9	-7.2	-7.7	-8.1	0.00%	0.00%	0.00%
Tralomethrin		66841-25-6	66841256	5167	Pest_427	6395	0.31	1.35	36	-2.41	1.02		-7.3	-7.8	-8.4	0.00%	0.00%	0.00%
Flucythrinate		70124-77-5	70124775	811	Pest_223	6396	-0.04	1.35	80	-1.04	1.35		-7.5	-7.8	-8.2	0.00%	0.00%	0.00%
Fenpyroximate		134098-61-6	134098616	429	Pest_61	6397	0.81	0.73	11	-0.30	0.55	4	-7.3	-7.8	-8.6	0.00%	0.00%	0.00%
Tau-fluvalinate		102851-06-9	102851069	157	Pest_10	6398	-0.05	1.35	28	-1.38	1.35		-7.4	-7.8	-8.2	0.00%	0.00%	0.00%
Bioresmethrin		28434-01-7	28434017	581	Pest_139	6399	0.22	1.35	16	-0.37	1.35		-7.4	-7.8	-8.2	0.00%	0.00%	0.00%
Resmethrin		10453-86-8	10453868	1114	Pest_410	6400	0.58	0.92	25	-0.16	0.83	4	-7.4	-7.8	-8.2	0.00%	0.00%	0.00%
Lambda-Cyhalothrin		91465-08-6	91465086	5001	Pest_366	6401	0.04	1.34	24	-0.34	1.84	7	-7.7	-7.9	-8.8	0.00%	0.00%	0.00%
Esfenvalerate		66230-04-4	66230044	786	Pest_212	6402	0.03	1.33	17	-0.44	0.86	24	-7.8	-7.9	-8.4	0.00%	0.00%	0.00%
Fenvalerate		51630-58-1	51630581	1111	Pest_347	6403	0.64	1.20	70	1.61	1.83	14	-7.8	-7.9	-8.4	0.00%	0.00%	0.00%
Buprofezin		953030-84-7	953030847	4866	Pest_296	6404	2.77	0.44	3				-8.0	-7.9	-9.2	0.00%	0.00%	0.00%
Acrinathrin		101007-06-1	101007061	4829	Pest_284	6405	0.86	2.36	3				-7.8	-7.9	-8.6	0.00%	0.00%	0.00%
Imazaquin		81335-37-7	81335377	4977	Pest_363	6406	5.57	0.17	4	4.79	0.17		-7.2	-7.9	-9.4	0.00%	0.00%	0.00%
Iodosulfuron		185119-76-0	185119760	4980	Pest_364	6407	4.24	1.35	3				-7.3	-8.0	-9.5	0.00%	0.00%	0.00%
Hexythiazox		78587-05-0	78587050	4974	Pest_362	6408	3.11	0.90	7	2.11	0.90		-7.4	-8.1	-9.1	0.00%	0.00%	0.00%

SUBSTANCE IDENTIFICATION							TOXICITY INFORMATION						EXPECTED IMPACT in 'EU WATER'					
Substance name	EC nr	CAS nr	CAS#	MLoS no	MLoS code	SBT nr	µEC50 [ug/L]	σEC50 [ug/L]	#Spec	µNOEC [ug/L]	σNOEC [ug/L]	#Spec	Z(Cwlocal) [·]	Z(Cwfresh) [·]	Z(Cwcoast) [·]	TP(Cwlocal) [-]	TP(Cwfresh) [-]	TP(Cwcoast) [-]
Primisulfuron		113036-87-6	113036876	5103	Pest_397	6409	3.18	1.50	3				-7.5	-8.1	-9.9	0.00%	0.00%	0.00%
Tefluthrin		79538-32-2	79538322	922	Pest_239	6410	-0.39	1.19	9	-1.39	1.35		-8.2	-8.1	-9.3	0.00%	0.00%	0.00%
Flucycloxuron		113036-88-7	113036887	4955	Pest_352	6411	1.18	1.24	3				-7.4	-8.1	-8.8	0.00%	0.00%	0.00%
Triflusulphuron		135990-29-3	135990293	5179	Pest_432	6412	3.39	1.45	3				-7.6	-8.4	-9.8	0.00%	0.00%	0.00%
Flubenzimine		37893-02-0	37893020	2810	Pest_164	6413	1.07	0.43	3				-8.8	-8.7	-9.8	0.00%	0.00%	0.00%
Prohexadione		88805-35-0	88805350	5104	Pest_398	6414	5.96	1.83	3				-8.7	-9.2	-11.1	0.00%	0.00%	0.00%
Abamectin		71751-41-2	71751412	1097	Pest_281	6415	1.43	1.69	13	2.19	3.07	3	-9.3	-9.3	-10.1	0.00%	0.00%	0.00%
Diafenthiuron		80060-09-9	80060099	4893	Pest_320	6416	1.27		2				-9.1	-9.4	-10.0	0.00%	0.00%	0.00%