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Environmental impacts of certain phthalates and alternatives to phthalates

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Environmental impacts of certain phthalates and alternatives to phthalates
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Content

Preface

This project ”Environmental impacts of certain phthalates and alternatives to phthalates” was carried out during the period from July 2013 to December 2013.

The objective of this project was to create an overview of the environmental effects of phthalates and their alternatives in order to help the industry and importers to select alternatives to the most problematic phthalates classified as toxic for the reproduction including the four phthalates DEHP, BBP, DBP and DIBP.

The project was implemented by DHI by a project team consisting of Anne Rathmann Pedersen (project manager), Morten Bjergstrøm and Dorte Rasmussen.

The project was advised by a steering committee consisting of Frank Jensen and Magnus Løfstedt, The Danish EPA, and Anne Rathmann Pedersen, DHI.

Summary and conclusion

Phthalates are widely used as softener in PVC and in the manufacture of materials. Phthalates are in focus because of their reproductive and endocrine disrupting effects. A number of phthalates, including the four phthalates DEHP, BBP, DBP and DIBP listed on the Authorisation List under REACH, are considered as harmful for reproduction and are classified as toxic for the reproduction. However, the group of phthalates represents a range of substances of different structure and different properties.

In spite of the extensive work carried out over the past 10-20 years on alternatives to phthalates of concern, the environmental and health effects of the alternatives still need to be reviewed. This includes substances within the group of phthalates but also alternative substances or groups of substances that can replace the use of phthalates.

Denmark has developed a phthalate strategy illustrating where there is knowledge, and where there is lack of information. As the main focus point has been effects on health because of the phthalates' reproductive toxicity and endocrine disrupting properties, an overview of the environmental impacts is still lacking. With the REACH registrations of the phthalates and their alternatives, the industry's own data have been provided, and these data are expected to be updated by registrants when new information on both the environmental and health impacts are available as required by the REACH regulation.

The objective of this project is to create an overview of the environmental effects of phthalates and their alternatives in order to help the industry and importers to select alternatives to the most problematic phthalates classified as toxic for the reproduction including the four phthalates DEHP, BBP, DBP and DIBP.

The overview of the environmental effects of phthalates can be grouped into these bullet points:

- fate in the environment
- effects in the relevant environmental compartments
- indication of PBT-properties
- indications of endocrine disrupting properties
- releases (amounts and pathways) into the environment

A final list of phthalates (28 substances) to be included in this project was prepared on the basis of the list of REACH-registered substances, contact to the PVC Information Council Denmark and by consulting the SPIN database.

A total of ten alternative substances have been identified by the Danish EPA. Environmental profiles for the identified alternatives to phthalates were elaborated based on information from the REACH registration dossiers for the alternatives and reported in datasheets.

Available data on the environmental properties of the selected phthalates have been reviewed and reported in datasheets. Various data sources have been consulted: REACH registration dossiers including Chemical Safety Reports, US EPA ECOTOX (US EPA), public databases via e-ChemPortal. In addition, QSAR tools were used to screen the phthalates and their alternatives for PBT-properties (using the US EPA PBT-profiler tool) and for indication of endocrine disrupting effects of the phthalates and the alternative substances. For the latter, the Lipinski's rules of five (included in

OECD QSAR Toolbox) were applied to indicate if the substance is bioavailable, as only bioavailable substances are biological active. Also the OECD QSAR Toolbox was applied to list the potential metabolites from the substances, and to identify if these form monoesters. The background for doing this is that it is recognized that monoester from DEHP is the most likely cause for DEHP to have endocrine disrupting properties. Finally, the QSAR-tool EpiSuite was applied in few instances for retrieving physical-chemical and fate data and to a smaller extend for retrieving ecotoxicity data.

Overall, the water solubility of the phthalates is found to be low and they have a high octanol-water partition coefficient increasing almost linearly with number of carbon (N) ($\log K_{ow} \approx 0.39 \times N - 1.87; N \geq 8; R^2 = 0.88$). The same trend can be observed for the alternatives ($\log K_{ow} \approx 0.62 \times N - 5.97; N \geq 9; R^2 = 0.86$).

A relation between the octanol-water distribution coefficient (log K_{ow}) and the biodegradability exists. With a few exceptions, phthalates with a log K_{ow} value below approximately 10 are readily biodegradable and phthalates with a log K_{ow} values above 10 are inherently biodegradable. The same overall conclusion is valid for the alternatives to phthalates but the available data set is much smaller.

The reported effect concentrations are often exceeding the water solubility of the substance tested. This means that the determined toxicities are not necessarily caused by the dissolved substances, but can be a consequence of physical effects. From the reported data it can be seen that the aquatic toxicity of the phthalates tends to increase with the number of carbon in the substance.

None of the registered phthalates and their alternatives is assessed as being a PBT or a vPvB substance. One phthalate has PBT-properties according to the PBT-profiler, namely benzyl 3-isobutyryloxy-1-isopropyl-2,2-dimethylpropyl phthalate (CAS no 16883-83-3). No PBT-assessment is included in the REACH registration for this substance– however the registrant has (based on read-across) assessed the substance to be readily biodegradable.

15 of the 28 phthalates were screened not to be bioavailable (Lipinski) indicating a low potential for being biological active (e.g. to have endocrine disrupting properties). Eight of the 28 phthalates were screened to be bioavailable (Lipinski), and thus to have a potential for being biological active. By use of the OECD Toolbox, six of these eight phthalates were screened to form - among several metabolites - monoesters. The monoester metabolised from DEHP has been identified to cause the endocrine disrupting properties for DEHP. Using OECD QSAR Toolbox, none of these eight phthalates was found to be estrogenic receptor (ER) binding, which may cause a subsequent endocrine disruption. The Lipinski bioavailability was not calculated for the last five of the phthalates due to lack of structural information.

For all registered substances, the reported ERCs (Environmental Release Categories) in the REACH registration dossier were extracted from the dossier and can be seen in the datasheets for the substances. It was found that most of the substances are registered as being manufactured within EU, to be formulated into a mixture/matrix and to have one or more industrial end-uses. In addition, several of the substances are registered to have wide dispersive uses. Several of the substances are also incorporated into articles and have been assigned a wide-dispersive service life. In general, the largest emission fractions are from industrial end uses and from wide dispersive uses such as professional or consumer uses. Therefore, as the phthalates and their alternatives have been registered for these uses, significant releases of the phthalates and their alternatives are expected. The fraction of non-phthalate alternatives reported to have wide dispersive uses is slightly higher than the fraction of the 28 phthalates reported to have wide dispersive uses.

The distribution in the environment of the substances was calculated by use of EUSES. Only regional emission was considered, and the emission into air and into water was assumed to be

equal. The steady-state regional concentration in the various environmental compartments was found and converted into amounts by multiplying with the capacity (m^3 for air and water, kg wet weight for sediment and soil) of the various regional compartments. The distribution could then be found by dividing the amount in the various compartments by the total amount in all compartments. It was found that none of the phthalates and their alternatives tends to concentrate in water. The distribution to air is of some importance for the short chained phthalates like DEP and DMP, but not for any of the identified alternatives to phthalates. Most of the phthalates and identified alternatives tend to concentrate in sediment and soil.

When choosing alternatives to e.g. DEHP, only alternatives with better or equal environment profiles should be considered. Readily biodegradable alternatives can be found within the group of phthalates with a log K_{ow} below 10. These are represented by phthalates with a carbon number below 30. When considering the aquatic toxicity of the phthalates, the phthalates with a carbon number below 20 could be considered.

Conclusions

Environmental profiles for 28 phthalates and ten alternatives to phthalates (28 substances) have been elaborated and reported in separate datasheets. Overall, the water solubility of the phthalates is found to be low and the substances and their alternatives have a high octanol-water partition coefficient increasing almost linearly with the number of carbon. A relation between the octanol-water distribution coefficient (log K_{ow}) and the biodegradability exists. With a few exceptions, phthalates with a log K_{ow} value below approximately 10 are readily biodegradable and phthalates with a log K_{ow} values above 10 are inherently biodegradable. The same overall conclusion is valid for the alternatives to phthalates but the available data set is much smaller. There is a general problem with the reported ecotoxicity test data, as the reported effect concentrations often exceed the water solubility of the substance tested. This means that the determined toxicities are not necessarily caused by the dissolved substances, but can be a consequence of physical effects. From the reported data it can be seen that the aquatic toxicity of the phthalates tends to increase with the number of carbon in the substance. None of the registered phthalates and their alternatives is assessed as being a PBT or a vPvB substance. The PBT-profiler indicates that one substance may be a PBT substance. Eight of the 28 phthalates were screened to be bioavailable (Lipinski), and thus to have a potential for being biological active. Six of these eight phthalates may form monoesters, which may have endocrine disrupting properties. Phthalates and their alternatives have been registered for industrial end uses and wide dispersive uses, and therefore, significant releases of the phthalates and their alternatives into the environment are expected. The fraction of non-phthalate alternatives reported to have wide dispersive uses is slightly higher than the fraction of the 28 phthalates reported to have wide dispersive uses. This may be a result of that the substitution of use of the most hazardous phthalates (DEHP, BBP, DBP and DIBP) as e.g. softeners with one of the alternatives has been taken place for some years by now. It was found that none of the phthalates and their alternatives tends to concentrate in water. The distribution to air is of some importance for the short chained phthalates like DEP and DMP, but not for any of the identified alternatives to phthalates. Most phthalates and identified alternatives tend to concentrate in sediment and soil, which is also the case for DEHP.

When choosing alternatives to e.g. DEHP, alternatives with better or equal environment profiles should be considered and these are represented by phthalates with a carbon number below 20. In addition, a good dataset of equal or better data quality than for DEHP should be ensured for the alternative and the sediment and soil PNEC values for the alternative should be higher than or comparable to the PNEC values for DEHP.

1. Introduction

Phthalates are widely used as softener in PVC and in the manufacture of some other materials. Therefore, phthalates can be found in many different types of products and materials. Phthalates are in focus because of their reproductive and endocrine disrupting effects. The use of some phthalates is regulated for various types of products such as toys and childcare products, food-contact material and medical devices. Some of the phthalates are also regulated by the Authorisation scheme under REACH and included on the Candidate List as well as Annex XIV for authorisation.

A number of phthalates, including the four phthalates DEHP, BBP, DBP and DIBP listed on the Authorisation List under REACH, are considered as harmful for reproduction and are classified as toxic for the reproduction. Over the past 10-20 years, both nationally and at EU level mappings of phthalates and their alternatives have been prepared – including environmental and health assessments of the group of substances and their alternatives. In spite of the extensive work carried out, primarily at the authority level, the environmental and health effects of alternatives to the four phthalates on the Authorisation List still need to be reviewed. This includes substances within the group of phthalates but also alternative substances or groups of substances that can replace the use of phthalates. Denmark has developed a phthalate strategy illustrating where there is knowledge, and where there is lack of information. As the main focus point has been effects on health because of the phthalates' reproductive toxicity and endocrine disrupting properties, aggregated information about environmental impacts is still lacking. With the REACH registrations of the phthalates and their alternatives, the industry's own data have been provided, and these data are expected to be updated by registrants when new information on both the environmental and health impacts are available as required by the REACH regulation.

The objective of this project is to create an overview of the environmental effects of phthalates and their alternatives in order to help the industry and importers to select alternatives to the most problematic phthalates classified as toxic for the reproduction including the four phthalates DEHP, BBP, DBP and DIBP.

2. Identification of the most widely used phthalates

2.1 Introduction

This chapter describes the selection of the phthalates considered to be most widely used and which are considered relevant for further studies on their environmental properties.

2.2 Basic list

The phthalates already registered in REACH are assumed to be the most widely used phthalates. On this basis, the Danish EPA has compiled a list of a total of 28 phthalates. This list is further adjusted excluding the following phthalates:

1. Phthalates, which are registered solely as intermediates. These are identified in the ECHA database of chemical substances, ECHA_CHEM accessible via http://echa.europa.eu/web/guest/information-on-chemicals/registered-substances.
2. Phthalates, which are on the Candidate List or have a harmonized classification as toxic for reproduction category 1B as these substances are not considered to be long-time alternatives. This is examined by comparison of the substances on the Candidate List and/or the CLP Annex VI with the 28 substances on the list from the Danish EPA.

2.3 Consultation of the PVC Information Council Denmark

The PVC Information Council Denmark has been contacted in order to check if they are aware of additional phthalates, which should be included in study.

The PVC Information Council Denmark listed a range of alternatives to DEHP, BBP, DBP and DIBP. The alternatives are the phthalates DINP, DIDP, DPHP and DOTP, which all are included in the basic list. Other softeners that are used to some degree are adipates, trimellitates, chlorinated paraffins etc.

2.4 SPIN database

SPIN is a database on the use of substances in chemical products (and not articles) in the Nordic Countries. The database is based on data from the Product Registries of Norway, Sweden, Denmark and Finland.

The substances included in the SPIN-database (http://90.184.2.100/DotNetNuke/default.aspx) were consulted. All substances –excluding polymers - with a name including “dicarboxylic” and being a di-ester were listed together with their consumption in Denmark. The results from consulting the SPIN database are shown in Appendix A. Only one substance fulfilling these conditions were identified, namely “1,2-Benzenedicarboxylic acid, bis(2-methoxyethyl) ester (CAS-No: 117-82-8)”. However, this substance is listed on the Candidate List under REACH due to its toxicity to reproduction and the substance is therefore not included in this project.

2.5 Summary

A final list of phthalates (28 substances) to be included in this project was prepared on the basis of the list of REACH-registered substances, contact to the PVC Information Council Denmark and by consulting the SPIN database. The final list of selected phthalates is shown in Table 1.

TABLE 1
SELECTED PHTHALATES

Phthalate	CAS No	EINECS No
Diethyl phthalate (DEP)	84-66-2	201-550-6
Dimethyl phthalate (DMP)	131-11-3	205-011-6
Diallyl phthalate (DAP)	131-17-9	205-016-3
Diundecyl phthalate (DUP)	3648-20-2	222-884-9
Benzyl 3-isobutyryloxy-1-isopropyl-2,2-dimethylpropyl phthalate	16883-83-3	240-920-1
Diisotridecyl phthalate (DITP)	27253-26-5	248-368-3
Di-"isononyl" phthalate (DINP)	28553-12-0	249-079-5
Bis(2-propylheptyl) phthalate (DPHP)	53306-54-0	258-469-4
1,2-benzenedicarboxylic acid, benzyl C7-9-branched and linear alkyl esters	68515-40-2	271-082-5
1,2-benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters	68515-43-5	271-085-1
1,2-benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13-rich	68515-47-9	271-089-3
1,2-benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich	68515-48-0	271-090-9
1,2-benzenedicarboxylic acid, di-C9-11-branched alkyl esters, C10-rich	68515-49-1	271-091-4
1,2-benzenedicarboxylic acid, di-C6-10-alkyl esters	68515-51-5	271-094-0
1,2-benzenedicarboxylic acid, di-C8-10-alkyl esters	71662-46-9	275-809-7
Diundecyl phthalate, branched and linear (DIUP)	85507-79-5	287-401-6
1,2-benzenedicarboxylic acid, di-C16-18-alkyl esters	90193-76-3	290-580-3
Tetraammonium 5-(4-(7-amino-1-hydroxy-3-sulfonato-2-naphthylazo)-6-sulfonato-1-naphthylazo)isophthalate	-	405-130-5
2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl 3,4,5,6-tetrabromophthalate	20566-35-2	243-885-0
Methyl 5-nitrohydrogen isophthalate	1955-46-0	217-793-6
Dibutyl terephthalate (DBTP)	1962-75-0	217-803-9
Bis(2-ethylhexyl) terephthalate	6422-86-2	229-176-9
Bis(2,3-epoxypropyl) terephthalate	7195-44-0	230-565-0
1,4-benzenedicarboxylic acid, dimethyl ester, manuf. of, by-products from	68988-22-7	273-521-6

Phthalate	CAS No	EINECS No
A mixture of: sodium 5-[8-[4-[4-[4-[7-(3,5-dicarboxylatophenylazo)-8-hydroxy-3,6-disulfonatonaphthalen-1-ylamino]-6-hydroxy-1,3,5-triazin-2-yl]-2,5-dimethylpiperazin-1-yl]-6-hydroxy-1,3,5-triazin-2-ylamino]-1-hydroxy-3,6-disulfonatonaphthalen-2-ylazo]-isophthalate; ammonium 5-[8-[4-[4-[4-[7-(3,5-dicarboxylatophenylazo)-8-hydroxy-3,6-disulfonatonaphthalen-1-ylamino]-6-hydroxy-1,3,5-triazin-2-yl]-2,5-dimethylpiperazin-1-yl]-6-hydroxy-1,3,5-triazin-2-ylamino]-1-hydroxy-3,6-disulfonatonaphthalen-2-ylazo]-isophthalate; 5-[8-[4-[4-[4-[7-(3,5-dicarboxylatophenylazo)-8-hydroxy-3,6-disulfonatonaphthalen-1-ylamino]-6-hydroxy-1,3,5-triazin-2-yl]-2,5-dimethylpiperazin-1-yl]-6-hydroxy-1,3,5-triazin-2-ylamino]-1-hydroxy-3,6-disulfonaphthalen-2-ylazo]-isophthalic acid	187285-15-0	413-180-4
Tetramethylammonium hydrogen phthalate	79723-02-7	416-900-5
Dimethyl terephthalate (DMTP)	120-61-6	204-411-8
Ester reaction products of 1,4-benzenedicarboxylic acid with C11-14 iso-alcohols, C13-rich		416-740-6

3. Environmental effects - methods

3.1 Introduction

Available data on the environmental properties of the selected phthalates have been reviewed. Various data sources have been consulted: REACH registration dossiers including Chemical Safety Reports, US EPA ECOTOX (US EPA), public databases via e-ChemPortal, original literature and the QSAR-tools EpiSuite and OECD QSAR Toolbox.

The various consulted data sources are briefly described in the following.

The data are stored in an Access database. Selected data from the database are extracted into standard word tables to form a datasheet for each individual phthalate (see Appendix B).

3.2 Environmental profile of the selected phthalates

The purpose of this review is to characterise the selected phthalates with respect to:

- fate in the environment
- effects in the relevant environmental compartments
- indication of PBT-properties
- indications of endocrine disrupting properties
- releases (amounts and pathways) into the environment

The environmental profile of the selected phthalates can be divided into the following main types:

Identification of the chemical

- CAS-number, EC-number and name
- Structure
- SMILES notation. In case of that the substance is not uniquely defined, e.g. it has a variable alkyl chain length, it is more or less branched, then an average SMILES notation has been assigned to the substance. For example if the substance is reported to have an alkyl chain length between 14 and 20, then the substance has been assigned a chain length of 17

Physical-chemical properties to identify the overall behaviour of the substances in the environment:

- Melting point and boiling point for the identification of the physical state of the substance in the environment (solid, liquid, vapour, gas)
- Octanol-water partition coefficient ($logK_{ow}$), vapor pressure and water solubility for an overall identification of which environmental compartments the phthalates tend to concentrate in

Fate properties:

- Biodegradability at aerobic conditions
- Water-air partition coefficient (Henrys constant, which can be estimated from vapour pressure and water solubility)
- Soil/sediment-water partition coefficient

Emission and exposure characteristics:

- Tonnage band based on registrations under REACH
- Lifecycle stages and ERCs (Environmental Release Categories – see ECHA guidance document on Information Requirements and Chemical Safety Assessment (R12) for more details
- EUSES predicted distribution of the phthalates in the environment

Ecotoxicity:

- Short-term (E(L)C50 mainly to algae, crustacean, fish and long-term (EC10 or NOEC/LOEC) mainly to algae, crustacean and fish

- Bioconcentration factors

Hazard profile

- PBT/vPvB-properties
- PNEC-values.
- CLP-classification

3.3 Data sources

The main data source was the REACH registration dossiers collected via ECHA's database ECHA-CHEM. ECHA-CHEM is accessible via http://echa.europa.eu/web/guest/information-on-chemicals/registered-substances.

If sufficient data could be retrieved from this data source, no further data search was carried out. Additional data search was carried out, if the substance was not REACH registered or if the REACH registration did not include all the required data.

3.3.1 REACH registration data

Relevant data from the public available registration dossiers for the identified phthalates have been reviewed. The review included the following from the registration dossiers:

- Classification and labelling
- PBT assessment
- Physical-chemical data: water solubility, vapour pressure, $\log K_{ow}$
- Environmental fate and pathways: (Readily) biodegradability at aerobic conditions, anaerobic biodegradability, Henrys law constant, K_{OC} and K_d values, BCF
- Ecotoxicological information both on pelagic and soil , i.e. E(L)C50, EC10, NOEC effect data on algae, crustacean and fish, and if available effect data on other species.
- Derived PNEC-values.

For each study, relevant information such as reliability (Klimisch score), test method, duration of test, organism, test conditions, results of testing and reference are listed. In addition, it is indicated, if data are based on "weight of evidence", read-across to other substances or QSAR.

The data listed above were, if available, extracted from key studies with the highest Klimisch scores as reported in the registration dossiers. For endpoints with no key studies available, data were extracted from non-key studies with the highest Klimisch scores. PNEC values are reported only when they were available in the registration dossiers. No further assessment of the data extracted from the registration dossiers was performed.

3.3.1.1 Chemical Safety Reports

Chemical Safety Reports (CSRs) for a number of classified and widely used phthalates have been received. The findings in the CSRs are reported in a separate confidential report.

3.3.2 US EPA ECOTOX

If needed, i.e. if ecotoxicity data are missing from the other data sources, supplementary data were retrieved from the US EPA database ECOTOX, which contains effect data (both water and soil) as well as BCF-data.

The database is accessible from http://cfpub.epa.gov/ecotox/advanced_query.htm

3.3.3 e-ChemPortal (OECD)

e-ChemPortal is an internet-based portal for a number of public accessible databases. Besides the already mentioned ECHA database containing REACH registration dossiers, the following databases are included in the e-ChemPortal:

- EnviChem
- ESIS (old IUCLID data)
- HSDB (Hazardous Substance Data Bank)
- INCHEM (Chemical Safety Information from Intergovernmental Organizations – INCHEM)
- J-CHECK (Japan CHEmicals Collaborative Knowledge database)
- JECDB (Japan Existing Chemical Data Base)
- NICNAS (Australian National Industrial Chemicals Notification and Assessment Scheme)
- OECD SIDS IUCLID (OECD Existing Chemicals Screening Information Data Sets (SIDS) Database
- SIDS UNEP (OECD Initial Assessment Reports for HPV Chemicals including Screening Information Data Sets (SIDS))

e-ChemPortal is accessible from http://www.echemportal.org/echemportal/page.action?pageID=0

These databases provide data on physical-chemical properties, fate properties and ecotoxicity data of the chemical substances.

3.3.4 CLP-classification

ECHA's C&L Inventory (http://echa.europa.eu/information-on-chemicals/cl-inventory) was consulted for CLP-self-classification data. Different CLP-classifications for the same substance may be found. In these cases, the classification and number of notifiers for each set of CLP-classification was noted.

3.3.5 PBT-profiler

The PBT-profiler is an internet-based QSAR-based screening level predictive tool designed to identify PBT chemicals that potentially may persist, bioaccumulate, and be toxic to aquatic life. The PBT-profiler predicts the

- P: half-lives in soil, water and air
- B: BCF (fish)
- T: the so-called chronic value to fish. The Chronic Value (ChV) is defined as the geometric mean of the no observed effect concentration (NOEC) and the lowest observed effect concentration (LOEC).

These predictions are compared to the PBT criteria and the output from the program is a predicted PBT-profile of the chemical. Input to the program is the SMILES notation.

The PBT-profiler is accessible from http://www.pbtprofiler.net/about.asp

The results from the PBT-profiler are transferred to the substance datasheets (Appendix B). It should be noted that the results from the PBT-profiler may conflict with the PBT/vPvB assessment retrieved from the REACH registration dossier, which is also reported in the substance datasheets. In case of any conflict, it is recommended to rely on the data from the REACH registration dossier, as the data here may be experimentally determined and have been subject for quality evaluation.

3.3.6 OECD QSAR Toolbox

The OECD QSAR Toolbox was used to predict if the phthalates have properties indicating a potential for endocrine disrupting properties.

For this purpose the following predictions from the OECD QSAR Toolbox were used:

- Bioavailability predicted by Lipinski's rules. Lipinski's Rule of Five is used to determine if a chemical compound has properties that would make it a likely orally active drug in humans. The rule describes molecular properties important for a drug's pharmacokinetics in the human body, including their absorption, distribution, metabolism, and excretion ("ADME"). The Lipinski's rule does not predict if a compound is pharmacologically active.
- Observed metabolism (mammalian, rat in vivo), rat liver S9 (observed and simulated) metabolism, microbial metabolism (observed and simulated) and their formed metabolites with an indication of if they are bioavailable (Lipinski's Rule of Five). It is checked if monoesters are formed according to the predictions/observation in the toolbox.

3.4 Emission into and distribution in the environment

3.4.1 Emission characteristics

For all registered substances, the reported ERCs in the REACH registration dossier were extracted from the dossier and can be seen in the datasheets for the substances. The ERCs were divided into the following categories for the profiling of their emission characteristics (Table 2).

TABLE 2
ERC GROUPING

Manufacture	Formulation	Industrial end-use (opened/closed)	Industrial end-use (closed)	Wide-dispersive end-use (opened/closed)	Wide-dispersive end-use (closed)	Service life (opened/closed)	Service life (closed)
ERC 1	ERC 2	ERC 4	ERC 7	ERC 8a	ERC 9a	ERC 10a	ERC 12a
	ERC 3	ERC 5		ERC 8b	ERC 9b	ERC 10b	ERC 12b
		ERC 6a		ERC 8c		ERC 11a	
		ERC 6b		ERC 8d		ERC 11b	
		ERC 6c		ERC 8e			
		ERC 6d		ERC 8f			

3.4.2 Distribution in the environment

The distribution in the environment of the substances was calculated by use of EUSES. Only regional emission was considered, and the emission into air and into water was assumed to be equal. The steady-state regional concentration in the various environmental compartments was then found by the calculation by EUSES. These steady-state concentrations were converted into amounts by multiplying with the capacity (m^3 for air and water, kg wet weight for sediment and soil) of the various regional compartments. The distribution could then be found by dividing the amount in the various compartments by the total amount in all compartments together.

4. Environmental properties of alternatives - methods

In total, ten alternatives to phthalates have been identified by the Danish EPA (Table 3).

TABLE 3
IDENTIFIED ALTERNATIVES TO PHTHALATES

Substance name		CAS No.	EINECS No.
Sulfonic acids, C10-21-alkane, Ph esters	**ASE**	91082-17-6	293-728-5
Acetyl tributyl citrate	**ATBC**	77-90-7	201-067-0
Glycerides, castor-oil mono-, hydrogenated, acetates	**COMGHA**	736150-63-3	451-530-8
Diethylene glycol dibenzoate	**DEGD**	120-55-8	204-407-6
Dioctyl terephthalate	**DEHT**	6422-86-2	229-176-9
Oxydipropyl dibenzoate	**DGD**	27138-31-4	248-258-5
Diisononyl adipate	**DINA**	33703-08-1	251-646-7
Diisononyl cyclohexane-1,2-dicarboxylate	**DINCH**	166412-78-8	431-890-2
Triacetin	**GTA**	102-76-1	203-051-9
2,2,4-trimethyl-1,3-pentanediol diisobutyrate	**TXIB**	6846-50-0	229-934-9

A review of available data on the environmental effects on these alternatives has been prepared. The same data sources as was used for the phthalates have been consulted, primarily data from REACH registration (ECHA-CHEM). The data are stored in an Access database. Selected data from the database are extracted into standard word tables to form a datasheet for each individual alternative to phthalates (see Appendix C).

Dioctyl terephthalate (DEHT) is also on the list of the selected phthalates (Bis(2-ethylhexyl) terephthalate CAS 6422-86-2). Therefore the data for this substance are only provided as part of the data for the selected phthalates.

5. Results and discussions

5.1 Fate and ecotoxicity data

In Tables 4-7, an overview of environmental fate data and ecotoxicity data is given for selected phthalates and alternatives to phthalates.

The phthalates have high octanol-water partition coefficients (log K_{ow}) which increase almost linearly with the number of carbon atoms (N) ($\log K_{ow} \approx 0.39 \times N - 1.87; N \geq 8; R^2 = 0.88$). The same trend can be observed for the alternatives ($\log K_{ow} \approx 0.62 \times N - 5.97; N \geq 9; R^2 = 0.86$) (see Figures 1 and 2).

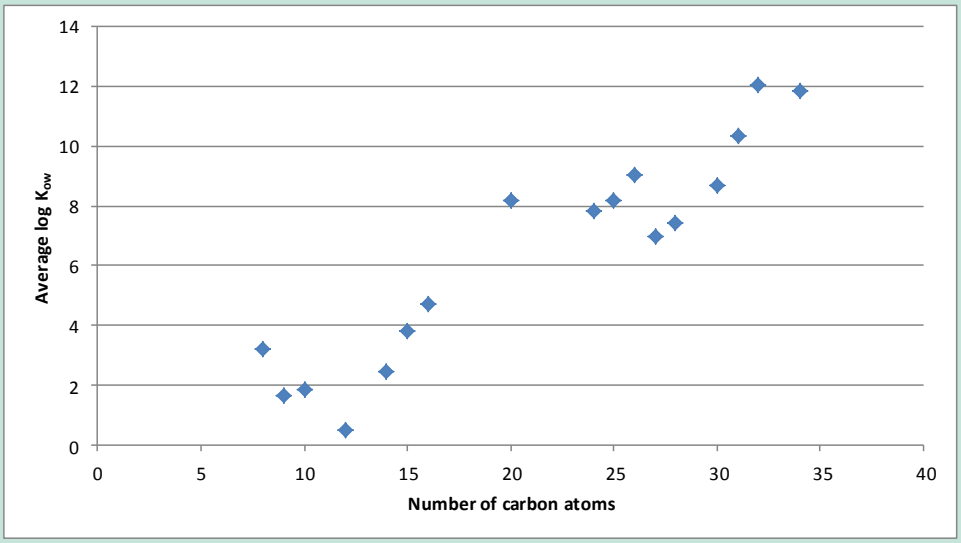

FIGURE 1
CORRELATION BETWEEN AVERAGE LOG K_{OW} AND NUMBER OF CARBON ATOMS FOR THE PHTHALATES

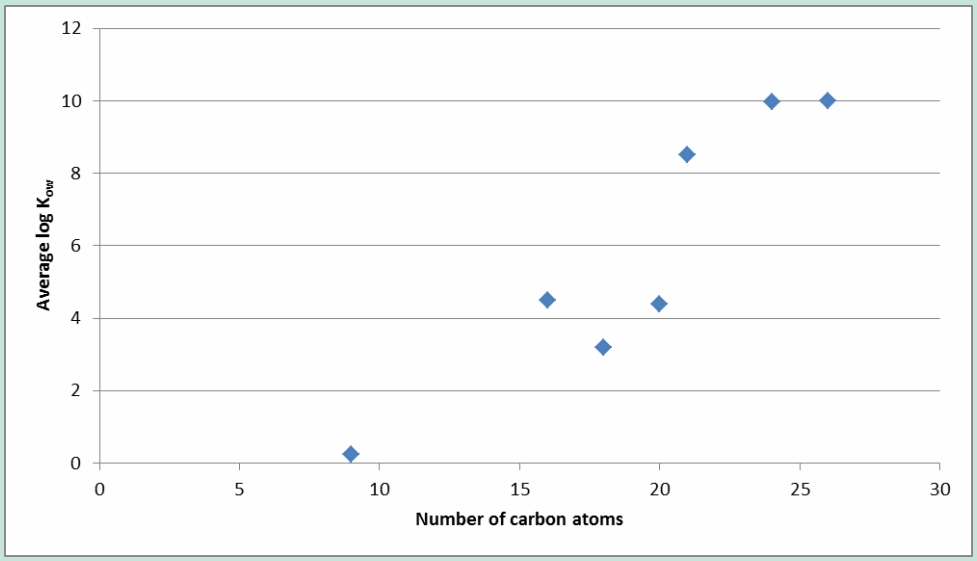

FIGURE 2
CORRELATION BETWEEN AVERAGE LOG K_{OW} AND NUMBER OF CARBON ATOMS FOR THE ALTERNATIVES TO PHTHALATES

For the phthalates it can be observed that a relation between the octanol-water distribution coefficient (log K_{ow}) and the biodegradability exists. With a few exceptions, phthalates with a log K_{ow} value below approx. 10 are readily biodegradable and phthalates with a log K_{ow} values above 10 are inherently biodegradable. For comparison, DEHP is readily biodegradable with a log K_{ow} below 10 (See Appendix D). The same overall conclusion is valid for the alternatives to phthalates but the available data set is much smaller and the group of alternative substances have a much more diverse chemical structure.

Overall, the water solubility of the phthalates is low and it is observed that the reported effect concentrations are often exceeding the water solubility of the substances tested (marked with stars in Tables 5 and 7) meaning that the determined toxicities are not necessarily caused by the dissolved substances, but can be a consequence of physical effects. Furthermore from Tables 5 and 7, it can be seen that most data on the effect concentrations EC50, LC50 and NOEC values are not reported with an exact value but given as a minimum concentration that does not exhibit toxic effects.

However, from the ecotoxicity data reported with scientifically valid effect concentrations, which are concentrations within the water solubility and with an exact value it can be seen that the aquatic toxicity of the phthalates tends to increase with the number of carbon (see Table 8). For comparison, the effect concentrations of DEHP are reported to be higher than the water solubility of DEHP, with acute EC50 of 0.1-0.2 mg/L and chronic NOEC of 0.2 mg/L for crustaceans (See Appendix D). When choosing alternatives to DEHP, the phthalates with a carbon number below 20 should be considered when comparing data on the aquatic toxicity of the phthalates.

For the terrestrial toxicity, no conclusions can be made as the data set is very limited (see Table 9). As the phthalates and their alternatives tend to concentration in sediment and soil, it is considered relevant to compare the PNECs for sediment (fresh water sediment) respectively soil. For reference and comparison these PNECs should also be compared with the PNECs for DEHP. Figures 3, 4 and 5 show the log K_{ow}, PNEC(fresh water sediment) and PNEC(soil) as a function of number of carbon atoms. Both phthalates and their non-phthalate alternatives are included in the figures.

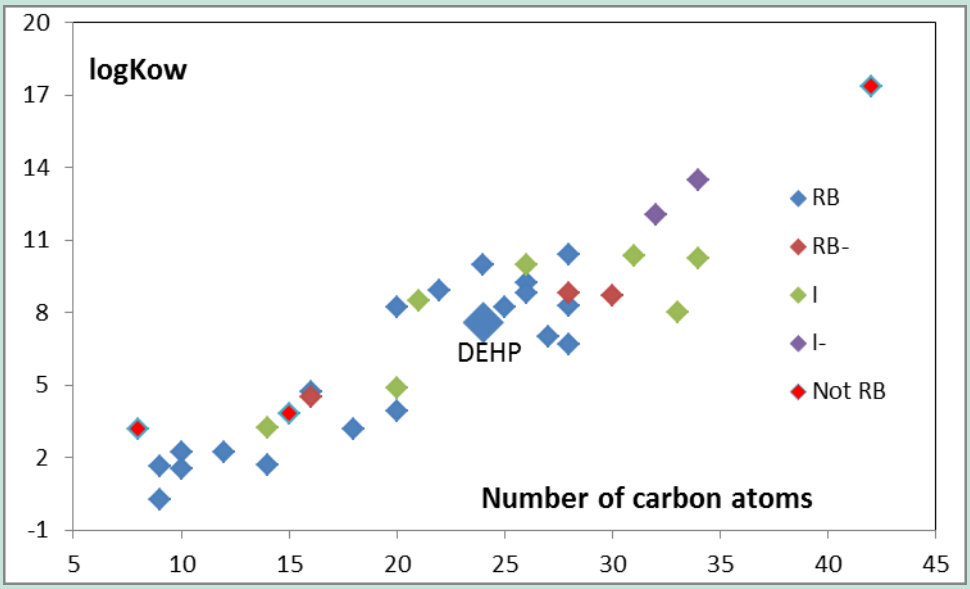

FIGURE 3
CORRELATION BETWEEN AVERAGE LOG K_{OW} AND NUMBER OF CARBON ATOMS. THE AEROBIC BIODEGRADABILITY FOR THE SUBSTANCES IS INDICATED. RB: READILY BIODEGRADABLE. RB-: READILY BIODEGRADABLE, NOT PASSING 10-D WINDOW; I: INHERENTLY BIODEGRADABLE; I-: INHERENTLY BIODEGRADABLE NOT FULFILLING CRITERIA. NOT RB: NOT READILY BIODEGRADABLE. THE PROPERTY OF DEHP IS INDICATED BY THE ENLARGED MARKER

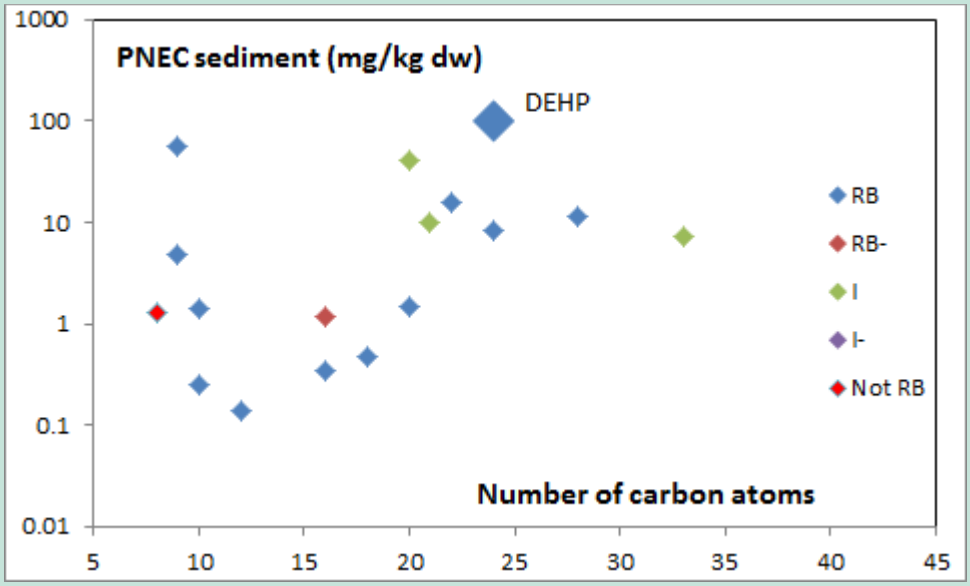

FIGURE 4
CORRELATION BETWEEN PNEC (FRESH WATER SEDIMENT) AND NUMBER OF CARBON ATOMS. THE AEROBIC BIODEGRADABILITY FOR THE SUBSTANCES IS INDICATED. RB: READILY BIODEGRADABLE. RB-: READILY BIODEGRADABLE, NOT PASSING 10-D WINDOW; I: INHERENTLY BIODEGRADABLE; I-: INHERENTLY BIODEGRADABLE NOT FULFILLING CRITERIA. NOT RB: NOT READILY BIODEGRADABLE. THE PROPERTY OF DEHP IS INDICATED BY THE ENLARGED MARKER. THE PHTHALATE DIALLYL PHTHALATE (DAP) IS OMITTED FROM THE FIGURE, AS IT HAS A VERY LOW PNEC VALUE.

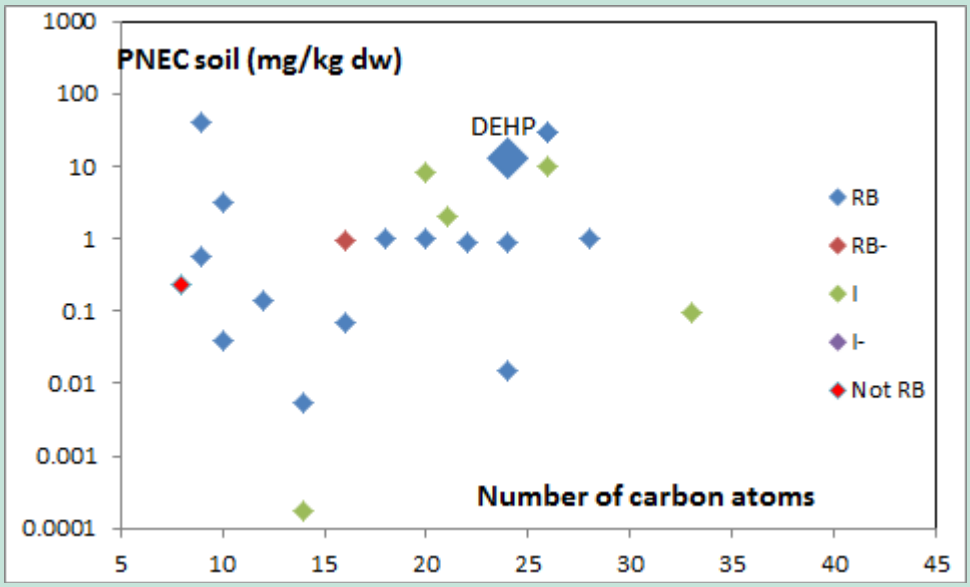

FIGURE 5
CORRELATION BETWEEN PNEC (SOIL) AND NUMBER OF CARBON ATOMS. THE AEROBIC BIODEGRADABILITY FOR THE SUBSTANCES IS INDICATED. RB: READILY BIODEGRADABLE. RB-: READILY BIODEGRADABLE, NOT PASSING 10-D WINDOW; I: INHERENTLY BIODEGRADABLE; I-: INHERENTLY BIODEGRADABLE NOT FULFILLING CRITERIA. NOT RB: NOT READILY BIODEGRADABLE. THE PROPERTY OF DEHP IS INDICATED BY THE ENLARGED MARKER

It is recognised that the PNEC values shown are a combination of the inherent toxicity and the quality and quantity of the dataset as safety assessment factors are applied to compensate for limited datasets. For many of the phthalates and the non-phthalate alternatives a high assessment factor is applied for the derivation of the soil and sediment PNEC values (using either soil and sediment ecotoxicity data (if available) or aquatic ecotoxicity data (if no soil and sediment ecotoxicity data is available and therefore the equilibrium partitioning method is used to derive the soil and sediment PNEC values)). For DEHP, the soil and sediment dataset is of high quality and a low assessment factor of 10 is applied for the sediment PNEC and for the soil PNEC values.

When choosing alternatives to e.g. DEHP, only alternatives with better or similar environment profiles should be considered. Readily biodegradable alternatives can be found within the group of phthalates with a log K_{ow} below 10. These are represented by phthalates with a carbon number below 30 (Figures 1 and 3). It should be noted that DEHP is registered as being readily biodegradable. From Figure 4 and 5, it appears that DEHP will have lower impact on the fresh water sediment and soil environments than most of the other phthalates and non-phthalate alternatives, as the PNECs for DEHP in general are higher than those for the other phthalates and non-phthalate alternatives. As mentioned above, this may be a result of limited dataset and thus high assessment factors applied for the phthalates and non-phthalate alternatives. Therefore, when considering substitution of DEHP with alternative substances, a good dataset of equal or better data quality than for DEHP should be ensured for the alternative and the sediment and soil PNEC values for the alternative should be higher than or comparable to the PNEC values for DEHP.

TABLE 4
ENVIRONMENTAL FATE DATA ON PHTHALATES (DATA ARE COLLECTED MAINLY FROM ECHA-CHEM, SEE INDIVIDUAL DATASHEETS FOR REFERENCES APPENDIX B)

Substance	CAS No.	PBT assessment	Biodegradability	Water solubility	log K_{ow}	Vapour pressure (Pa)	Kh (Pa m^3/mol)	K_{oc}
1,2-benzenedicarboxylic acid, benzyl C7-9-branched and linear alkyl esters	68515-40-2	-	Readily biodegradable (OECD Guideline 301 B)	0.00979 mg/L	6.66	0.000117	-	log K_{OC}: 3.974
1,2-benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13-rich	68515-47-9	The sub-stance is not PBT / vPvB	Inherently biodegradable, not fulfilling specific criteria (OECD Guideline 301 F)	0.00007 µg/L	12.06	0.0000000363	275	log K_{OC}: 6.08
1,2-benzenedicarboxylic acid, di-C16-18-alkyl esters	90193-76-3	The sub-stance is not PBT / vPvB	Not readily biodegradable (OECD Guideline 301 B)	<0.05 mg/L	17.38	1.61xE-20	-	log K_{OC}: 10.4
1,2-benzenedicarboxylic acid, di-C6-10-alkyl esters	68515-51-5	-	Readily biodegradable (EU Method C.4-C (Determination of the Ready Biodegradability - Carbon Dioxide Evolution Test))	11 mg/L	8.2	<0.1	0.901	log K_{OC} (first main component): 5.55, ; log K_{OC} (second component): 7.6

Substance	CAS No.	PBT assessment	Biodegradability	Water solubility	log K_{ow}	Vapour pressure (Pa)	Kh (Pa m^3/mol)	K_{oc}
1,2-benzenedicarboxylic acid, di-C8-10-alkyl esters	71662-46-9	-	Readily biodegradable (EU Method C.4-C (Determination of the ""Ready"" Biodegradability - Carbon Dioxide Evolution Test))	Approx. 0.00005572 mg/L	8.2	<0.1	1.01	log K_{OC}: 5.409
1,2-benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich	68515-48-0	The sub-stance is not PBT / vPvB	Readily biodegradable (OECD Guideline 301 F)	0.6 µg/L	8.8	ca. 0.00006	41.4	log K_{OC}: 5.9
1,2-benzenedicarboxylic acid, di-C9-11-branched alkyl esters, C10-rich	68515-49-1	The sub-stance is not PBT / vPvB	Readily biodegradable, but failing 10-day window (OECD Guideline 301 F)	0.00017 mg/L	8.8	0.000051	114	log K_{OC}: 5.46
1,2-benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters	68515-43-5	-	Readily biodegradable (EU Method C.4-C Determination of the Ready Biodegradability - Carbon Dioxide Evolution Test; OECD Guideline 301 B)	0.9385 µg/L	8.3	0.0357	3.72	log K_{OC}: 5.3849

Substance	CAS No.	PBT assessment	Biodegradability	Water solubility	log K_{ow}	Vapour pressure (Pa)	Kh (Pa m^3/mol)	K_{OC}
1,4-benzenedicarboxylic acid, dimethyl ester, manuf. Of, by-products from	68988-22-7	The sub-stance is not PBT / vPvB	Not readily biodegradable (OECD Guideline 301 B)	<0.983 mg/L	3.2	0.536	-	log K_{OC}: 1.624 - 2.962
2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl 3,4,5,6-tetrabromophthalate	20566-35-2	The sub-stance is not PBT / vPvB	The reference substance is not expected to be readily biodegradable (EPIwin)	0.05697 mg/L	3.8256	3.16E-12	2.26E-016	K_{OC}: 10
A mixture of: sodium 5-[8-[4-[4-[4-[7-(3,5-dicarboxylatophenylazo)-8-hydroxy-3,6-disulfonato-naphthalen-1-ylamino]-6-hydroxy-1,3,5-triazin-2-yl]-2,5-dimethylpiperazin-1-yl]-6-hydroxy-1,3,5-triazin-2-ylamino]-1-hydroxy-3,6-disul-fonatonaphthalen-2-ylazo]-isophthalate; (name shortened)	187285-15-0	-	-	-	-	-	-	-
Benzyl 3-isobutyryloxy-1-isopropyl-2,2-dimethylpropyl phthalate	16883-83-3	-	Readily biodegradable (OECD Guideline 301 B)	0.00147 mg/L	7	0.000000848	-	log K_{OC}: 4.666
Bis(2,3-epoxypropyl) terephthalate	7195-44-0	-	Readily biodegradable (OECD Guideline 301 F)	77 mg/L	1.7	<= 0.0000678	-	log K_{OC}: 2

Substance	CAS No.	PBT assessment	Biodegradability	Water solubility	log K_{ow}	Vapour pressure (Pa)	Kh (Pa m^3/mol)	K_{OC}
Bis(2-ethylhexyl) terephthalate	6422-86-2	The sub-stance is not PBT / vPvB	Readily biodegradable (OECD Guideline 301 B)	Approx. 0.4 µg/L	7.81	<0.001	-	log K_{OC}: 5.43
Bis(2-propylheptyl) phthalate (DPHP)	53306-54-0	The sub-stance is not PBT / vPvB	Readily biodegradable (OECD Guideline 301 B)	<0.0001 mg/L	>6	0.0000037	3.72	log K_{OC}: >5.63
Diallyl phthalate (DAP)	131-17-9	-	Inherent, ultimate biodegradable (OECD Guideline 302 C)	0.148 g/L	3.23	0.15	0.039	K_{OC}: 429
Dibutyl terephthalate (DBTP)	1962-75-0	The sub-stance is not PBT / vPvB	Readily biodegradable (OECD Guideline 301 B)	0.00451 mg/L	4.74	<0.038	-	log K_{OC}: 3.85
Diethyl phthalate (DEP)	84-66-2	The sub-stance is not PBT / vPvB	Readily biodegradable (US EPA 1982, Chemical fate test guidelines EPA560/6-82-003 US environmental protection agency Washington DC USA)	932 mg/L	2.2	<2800	0.0399	log $K_{OC,soil}$: 2.34

Substance	CAS No.	PBT assessment	Biodegradability	Water solubility	log K_{ow}	Vapour pressure (Pa)	Kh (Pa m^3/mol)	K_{OC}
Di-"isononyl" phthalate (DINP)	28553-12-0	Not P/vP, not B/vB, not T	Readily biodegradable (EU Method C.4-C Determination of the Ready Biodegrad-ability - Carbon Dioxide Evolution Test)	0.6 µg/L	8.8 - 9.7	0.00006	41.4	log K_{OC}: 6
Diisotridecyl phthalate (DITP)	27253-26-5	-	Inherently biodegradable, not fulfilling specific criteria (OECD Guideline 301 F)	Insoluble	13.5	<0.001	275	log K_{OC}: 6.08
Dimethyl phthalate (DMP)	131-11-3	Not vPvB; not T	Readily biodegradable (OECD Guideline 301 E)	4,000 mg/L	1.54	0.13	0.023	K_{OC}: 37.09
Dimethyl terephthalate (DMTP)	120-61-6	The sub-stance is not PBT / vPvB	Readily biodegradable (ISO Draft (BOD Test for Insoluble Substances))	31 mg/L	2.21	0.139	0.870696	K_{OC}: 30.96

Substance	CAS No.	PBT assessment	Biodegradability	Water solubility	log K_{OW}	Vapour pressure (Pa)	Kh (Pa m^3/mol)	K_{OC}
Diundecyl phthalate (DUP)	3648-20-2	-	Readily biodegradable, but failing 10-day window (EU Method C.4-C (Determination of the Ready Biodegrad-ability - Carbon Dioxide Evolution Test))	1.11 mg/L	8.7	<700	5.68	log $K_{OC,soil}$: 21.41
Diundecyl phthalate, branched and linear (DIUP)	85507-79-5	The sub-stance is not PBT / vPvB	Inherently biodegradable (OECD Guideline 301 F)	0.00441 µg/L	10.33	0.000000497	50.5	log K_{OC}: > 5.46 < 6.08
Ester reaction products of 1,4-benzenedicarboxylic acid with C11-14 iso-alcohols, C13-rich	-	-	Inherently biodegradable (OECD Guideline 301 B)	>0.000026 <0.00068 mg/L	>= 9.5 <= 11	0.00042	4296	log K_{OC}: 8.15
Methyl 5-nitrohydrogen. isophthalate	1955-46-0	-	Readily biodegradable (BIOWIN (v4.10))	1,900 mg/L	1.65	0.0000114	1.30E-007	K_{OC}: 11.846
Tetraammonium 5-(4-(7-amino-1-hydroxy-3-sulfonato-2-naphthylazo)-6-sulfonato-1-naphthylazo)isophthalate	128351-36-0	-	-	-	-	-	-	-
Tetramethylammonium hydrogen phthalate	79723-02-7	-	Readily biodegradable (OECD Guideline 301 D)	725 g/L	-1.24	<= 0.00001	-	-

TABLE 5
ECOTOXICITY DATA ON PHTHALATES (DATA ARE COLLECTED MAINLY FROM ECHA-CHEM, SEE INDIVIDUAL DATASHEETS FOR REFERENCES APPENDIX B)

Substance	CAS No.	Algae	Crustaceans	Fish	Terrestrial
1,2-benzenedicarboxylic acid, benzyl C7-9-branched and linear alkyl esters	68515-40-2	EC50: > 1000 ppm*	LC50: 4.5 mg/L* NOEC: 0.039 mg/L	LC50: >1000 mg/L* MATC: 0.3 mg/L	-
1,2-benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13-rich	68515-47-9	EC50: >0.6 mg/L*	LC50: >0.05 mg/L* NOEC: 0.052 mg/L*	LC50: >0.15 mg/L* NOEC: 0.3 mg/L*	Plants: L[E]C50: >100 mg/kg soil dw Macroorganisms: LC50: >7664 mg/kg
1,2-benzenedicarboxylic acid, di-C16-18-alkyl esters	90193-76-3	EL50: >100%	EC0: >= 10,000 mg/L*	LC50: >100 mg/L*	-
1,2-benzenedicarboxylic acid, di-C6-10-alkyl esters	68515-51-5	EC50: >2.8 mg/L	EC50: >1.7 mg/L NOEC: 0.059 mg/L	LC50: >0.32 mg/L NOEC: 0.3 mg/L	Plants: LC50: > 100 mg/kg soil dw Macroorganisms: LC10: >1000 mg/kg soil dw
1,2-benzenedicarboxylic acid, di-C8-10-alkyl esters	71662-46-9	EC50: >0.83 mg/L*	EC50: >4.3 mg/L* NOEC: 0.059 mg/L*	LC50: >0.32 mg/L* NOEC: 0.3 mg/L*	Plants: L[E]50: >100 mg/kg soil dw Macroorganisms: LC10: >1000 mg/kg soil dw

Substance	CAS No.	Algae	Crustaceans	Fish	Terrestrial
1,2-benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich	68515-48-0	EC50: >1.8 mg/L*	EC50: >0.06 mg/L* NOEC: 0.0036 mg/L*	LC50: >0.52 mg/L* NOEC: >= 18.5 <= 24.5 other: ug/g feed	Plants: NOEC: 1018 g/kg artificial soil Macroorganisms: LC50: >7270 mg/kg natural soil d
1,2-benzenedicarboxylic acid, di-C9-11-branched alkyl esters, C10-rich	68515-49-1	EC50: >0.8 mg/L*	LC50: >0.02 mg/L* NOEC: 0.0034 mg/L*	LC50: >0.62 mg/L* NOEC: >= 19.2 <= 22.7 other: ug/g feed	Plants: EC50: 8551 mg/kg artificial soil Macroorganisms: LC50: >7664 mg/kg natural soil dw
1,2-benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters	68515-43-5	EC50: >0.83 mg/L*	EC50: > 4.3 mg/L* NOEC: 0.56 mg/L*	LC50: >0.32 mg/L* NOEC: 0.3 mg/L*	Plants: L[E]C50: > 100 mg/kg soil dw Macroorganisms: LC10: >1000 mg/kg soil dw
1,4-benzenedicarboxylic acid, dimethyl ester, manuf. Of, by-products from	68988-22-7	EC50: 3.2 mg/L*	EC50: 3.9 mg/L*	EC50: >1.4 mg/L*	-
2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl 3,4,5,6-tetrabromophthalate	20566-35-2	EC50: 0.849 mg/L*	EC50: 10.779 mg/L*	LC50: 12 mg/L* LC50: 1.116 mg/L*	-

Substance	CAS No.	Algae	Crustaceans	Fish	Terrestrial
A mixture of: sodium 5-[8-[4-[4-[4-[7-(3,5-dicarboxylatophenylazo)-8-hydroxy-3,6-disulfonatonaphthalen-1-ylamino]-6-hydroxy-1,3,5-triazin-2-yl]-2,5-dimethylpiperazin-1-yl]-6-hydroxy-1,3,5-triazin-2-ylamino]-1-hydroxy-3,6-disulfonatonaphthalen-2-ylazo]- isophthalate; (name shortened)	187285-15-0	-	-	-	-
Benzyl 3-isobutyryloxy-1-isopropyl-2,2-dimethylpropyl phthalate	16883-83-3	EC50: >1,000 ppm*	LC50: >7.5 mg/L*	LC50: >1000 mg/L*	-
Bis(2,3-epoxypropyl) terephthalate	7195-44-0	EC50: 1.13 mg/L NOEC: 0.327 mg/L	EC50: 81 mg/L*	LC50: 8.8 mg/L	-
Bis(2-ethylhexyl) terephthalate	6422-86-2	EC50: >0.86 mg/L*	EC50: >1.4 µg/L* NOEC: >= 0.76 µg/L*	LC50: >984 mg/L* NOEC: >=0.28 mg/L*	Plants: EC50: >1400 µg/L
Bis(2-propylheptyl) phthalate (DPHP)	53306-54-0	EC50: >100 mg/L*	EC50: >100 mg/L* NOEC: >1 mg/L*	LC50: >10000 mg/L*	-
Diallyl phthalate (DAP)	131-17-9	EC50: 3.8 mg/L	EC50: 5.5 mg/L NOEC: 3.2 mg/L	LC50: 0.24 mg/L	-

Substance	CAS No.	Algae	Crustaceans	Fish	Terrestrial
Dibutyl terephthalate (DBTP)	1962-75-0	EC50: >0.013 mg/L*	EC50: >0.34 mg/L* NOEC: >=50 µg/L*	LC50: >0.17 mg/L* NOEC: >=24 µg/L*	-
Diethyl phthalate (DEP)	84-66-2	EC50: 23 mg/L	LC50: 90 mg/L NOEC: 25 mg/L	LC50: 12 mg/L LOEC: >= 0.1 <= 1 mg/L	Plants: LC50: 134 mg/kg dry soil Macroorganisms: LC50: 0.85 mg/cm2
Di-"isononyl" phthalate (DINP)	28553-12-0	EC50: >88 mg/L*	EC50: >74 mg/L* NOEC: >101 mg/L*	LC50: > 102 mg/L* NOEC: >= 18.5 <= 24.5 µg/g feed	Plants: NOEC: 1000 mg/kg soil dw Macroorganisms: LC50: >7270 mg/kg natural soil dw
Diisotridecyl phthalate (DITP)	27253-26-5	EC50: >0.6 mg/L*	LC50: >0.05 mg/L NOEC: 0.052 mg/L	LC50: >0.15 mg/L* NOEC: 0.3 mg/L*	Plants: EC50: >8551 mg/kg artificial soil Macroorganisms: LC50: >8435 mg/kg soil dw
Dimethyl phthalate (DMP)	131-11-3	EC50: 204 mg/L	LC50: > 52 mg/L NOEC: 9.6 mg/L	LC50: 39 mg/L NOEC: 11 mg/L	Macroorganisms: LC50: 3160 mg/kg soil dw
Dimethyl terephthalate (DMTP)	120-61-6	EC50: >29 mg/L	EC50: >23.5 mg/L NOEC: 1.72 mg/L	LC50: 13 mg/L	-
Diundecyl phthalate (DUP)	3648-20-2	EC50: >3.3 mg/L*	EC50: >0.022 mg/L NOEC: 0.059 mg/L	LC50: 1.4 mg/L* NOEC: 0.3 mg/L	Plants: LC50: >100 mg/kg soil dw Macroorganisms: LC10: >1000 mg/kg soil dw

Substance	CAS No.	Algae	Crustaceans	Fish	Terrestrial
Diundecyl phthalate, branched and linear (DIUP)	85507-79-5	EC50: >2.1 mg/L*	EC50: >0.9 mg/L* NOEC: 0.9 mg/L*	LC50: >1.4 mg/L* NOEC: >= 19.2 <= 22.7 other: ug/g feed	Plants: EC50: >8551 other: mg/kg artificial soil Macroorganisms: LC50: >7664 other: mg/kg natural soil dw
Ester reaction products of 1,4-benzenedicarboxylic acid with C11-14 iso-alcohols, C13-rich	-	EL50: >5008 mg/L*	EL50: >5100 mg/L* NOEL: >1 µg/L*	LL50: >5008 mg/L* NOEL: >0.35 mg/L*	Plants: EL50: >1500 µg/L Macroorganisms: LL50: >10,000 mg/kg natural and artificial soil d.w.
Methyl 5-nitrohydrogen.isophthalate	1955-46-0	EC50: 24.85464 mg/L	EC50: 26.5849 mg/L ChV: 887.873 mg/L	EC50: 30.42095 mg/L LC50: 167,000 mg/L*	Plants: IC50: 27.44769 mg/L Macroorganisms: LC50: 41,695.367 mg/L
Tetraammonium 5-(4-(7-amino-1-hydroxy-3-sulfonato-2-naphthylazo)-6-sulfonato-1-naphthylazo)isophthalate	128351-36-0	EC50: 0.04 mg/L*	LC50: 0.362 mg/L* ChV: 0.0008 mg/L	LC50: 0.073 mg/L* ChV: 0.0002 mg/L*	-
Tetramethylammonium hydrogen phthalate	79723-02-7	EC50: 0.32 mg/L	EC50: 3.3 mg/L	-	-

* Toxicity concentration above water solubility

TABLE 6
ENVIRONMENTAL FATE DATA ON ALTERNATIVES TO PHTHALATES (DATA ARE COLLECTED MAINLY FROM ECHA-CHEM, SEE INDIVIDUAL DATASHEETS FOR REFERENCES APPENDIX C)

Substance	CAS No.	PBT assessment	Biodegradability	Water solubility	log K_{OW}	Vapour pressure (Pa)	Kh (Pa m^3/mol)	K_{OC}
1-isopropyl-2,2-dimethyltrimethylene diisobutyrate (TXIB)	6846-50-0	The substance is not PBT / vPvB	Readily biodegradable, but failing 10-day window (OECD Guideline 301 B)	12.7 mg/L	4.49	<1.5	-	log K_{OC}: 3.6
COMGHA	736150-63-3	-	Readily biodegradable (OECD Guideline 301 F)	< 0.33 mg/L	6.4	0.000000048	-	log K_{OC}: 5.4
Diisononyl adipate (DINA)	33703-08-1	The substance is not PBT / vPvB	Readily biodegradable (OECD Guideline 301 F)	0.0032 mg/L	9.56 - 10.4	0.0000002	9.210442	log K_{OC}: 5.291
DINCH	166412-78-8	-	Inherently biodegradable (no conclusion in dossier) (-)	<0.02 mg/L	10	0.000022	7.15	log K_{OC}: 6.59
Oxydiethylene dibenzoate (DEGD)	120-55-8	The substance is not PBT / vPvB	Readily biodegradable (EU Method C.4-C)	38.3 mg/L	3.2	0.000018	-	log K_{OC}: 3.2
Oxydipropyl dibenzoate (DGD)	27138-31-4	The substance is not PBT / vPvB	Readily biodegradable (EU Method C.4-C)	Approx. 8.69 mg/L	3.9	0.00016	-	log K_{OC}: 3.6

Substance	CAS No.	PBT assessment	Biodegradability	Water solubility	log K_{ow}	Vapour pressure (Pa)	Kh (Pa m^3/mol)	K_{oc}
Sulfonic acids, C10-21-alkane, Ph esters (ASE)	91082-17-6	-	C10-21-alkane, Ph esters is not readily biodegradable, but is degradable as the pass level of 60% degradation (BOD) was achieved after 47 days (EU Method C.4-D)	2.2 mg/L	5.7 - 11.3	0.000294	0.04 – 0.061	log K_{OC}: 4.5 - 9.3
Triacetin (GTA)	102-76-1	The sub-stance is not PBT / vPvB	Readily biodegradable (OECD Guideline 301 B)	58 g/L	0.25	0.3306	0.000177	log K_{OC}: 0.93
Tributyl O-acetylcitrate (ATBC)	77-90-7	The sub-stance is not PBT / vPvB	Inherently biodegrad-able	4.49 mg/L	4.86	0.0494	4.434	log K_{OC}: 4.271

TABLE 7
ECOTOXICITY DATA ON ALTERNATIVES TO PHTHALATES (DATA ARE COLLECTED MAINLY FROM ECHA-CHEM, SEE INDIVIDUAL DATASHEETS FOR REFERENCES APPENDIX C)

Substance	CAS No.	Algae	Crustaceans	Fish	Terrestrial
1-isopropyl-2,2-dimethyltrimethylene diisobutyrate (TXIB)	6846-50-0	EC50: >7.49 mg/L	EC50: >1.55 mg/L NOEC: 0.7 mg/L	NOEC: >=6 mg/L	-
COMGHA	736150-63-3	EC50: 106 mg/L*	EC50: 0.92 mg/L* NOEC: >=70 µg/L	LC50: >0.28 mg/L NOEC: 32.1 µg/L	Plants: EC50: 12.5 mg/kg soil dw Macroorganisms: LC50: >1000 mg/kg soil dw
Diisononyl adipate (DINA)	33703-08-1	EC50: >100 mg/L*	EC50: >100 mg/L* NOEC: >=0.77 mg/L*	LC50: >500 mg/L*	Macroorganisms: LC50: 865 mg/kg soil dw
DINCH	166412-78-8	EC50: >100 mg/L*	EC50: >100 mg/L* NOEC: >=0.021 mg/L*	LC50: >100 mg/L*	Plants: EC50: > 1000 mg/kg soil dw Macroorganisms: LC50: >1000 mg/kg
Oxydiethylene dibenzoate (DEGD)	120-55-8	EL50: 10.94 mg/L	EL50: 6.7 mg/L	LL50: 2.9 mg/L	Macroorganisms: LC50: >1000 ppm
Oxydipropyl dibenzoate (DGD)	27138-31-4	EL50: 4.9 mg/L	EL50: 19.3 mg/L*	LC50: 3.7 mg/L	Macroorganisms: LC50: >1000 ppm
Sulfonic acids, C10-21-alkane, Ph esters (ASE)	91082-17-6	EC0: >=2 mg/L	EC0: >=100 mg/L*	LC0: >=2 mg/L	-
Triacetin (GTA)	102-76-1	EC50: >940 mg/L	EC50: 380 mg/L NOEC: >= 94 mg/L	LC50: >100 mg/L LOEC: 100 mg/L	-

Substance	CAS No.	Algae	Crustaceans	Fish	Terrestrial
Tributyl O-acetylcitrate (ATBC)	77-90-7	EC50: 74.4 mg/L*	EC50: >1 mg/L NOEC: >=1.11 mg/L	LC50: >38 and <60 mg/L*	-

* Toxicity concentration above water solubility

TABLE 8
AQUATIC TOXICITY DATA ON PHTHALATES (DATA REPORTED WITH SCIENTIFICALLY VALID EFFECT CONCENTRATIONS)

Substance	Carbon number	Algae	Crustaceans	Fish
Methyl 5-nitrohydrogen.isophthalate	9	EC50: 24.85464 mg/L	EC50: 26.5849 mg/L	EC50: 30.42095 mg/L
Dimethyl phthalate (DMP)	10	EC50: 204 mg/L	NOEC: 9.6 mg/L	LC50: 39 mg/L NOEC: 11 mg/L
Dimethyl terephthalate (DMTP)	10		NOEC: 1.72 mg/L	LC50: 13 mg/L
Diethyl phthalate (DEP)	12	EC50: 23 mg/L	LC50: 90 mg/L NOEC: 25 mg/L	LC50: 12 mg/L
Tetramethylammonium hydrogen phthalate	12	EC50: 0.32 mg/L	EC50: 3.3 mg/L	-
Bis(2,3-epoxypropyl) terephthalate	14	EC50: 1.13 mg/L NOEC: 0.327 mg/L		LC50: 8.8 mg/L
Diallyl phthalate (DAP)	14	EC50: 3.8 mg/L	EC50: 5.5 mg/L NOEC: 3.2 mg/L	LC50: 0.24 mg/L
1,2-benzenedicarboxylic acid, di-C6-10-alkyl esters	20		NOEC: 0.059 mg/L	NOEC: 0.3 mg/L
1,2-benzenedicarboxylic acid, benzyl C7-9-branched and linear alkyl esters	28		NOEC: 0.039 mg/L	MATC: 0.3 mg/L
Diundecyl phthalate (DUP)	30		NOEC: 0.059 mg/L	NOEC: 0.3 mg/L
Diisotridecyl phthalate (DITP)	34		NOEC: 0.052 mg/L	

For comparison, the effect concentrations of DEHP are reported to be higher than the water solubility of DEHP, with acute EC50 of 0.1-0.2 mg/L and chronic NOEC of 0.2 mg/L for crustaceans (Appendix D).

TABLE 9
TERRESTRIAL TOXICITY DATA ON PHTHALATES (DATA REPORTED WITH SCIENTIFICALLY VALID EFFECT CONCENTRATIONS)

Substance	Carbon number	Terrestrial
Methyl 5-nitrohydrogen.isophthalate	9	Plants: IC50: 27.44769 mg/L Macroorganisms: LC50: 41,695.367 mg/L
Dimethyl phthalate (DMP)	10	Macroorganisms: LC50: 3160 mg/kg soil dw
Diethyl phthalate (DEP)	12	Plants: LC50: 134 mg/kg dry soil Macroorganisms: LC50: 0.85 mg/cm2
Di-"isononyl" phthalate (DINP)	26	Plants: NOEC: 1000 mg/kg soil dw
1,2-benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich	26	Plants: NOEC: 1018 g/kg artificial soil
1,2-benzenedicarboxylic acid, di-C9-11-branched alkyl esters, C10-rich	28	Plants: EC50: 8551 mg/kg artificial soil

5.1 PBT and vPvB properties

None of the registered phthalates and their alternatives is assessed as being a PBT or a vPvB substance. According to the PBT-profiler, one phthalate has PBT-properties, namely benzyl 3-isobutyryloxy-1-isopropyl-2,2-dimethylpropyl phthalate (16883-83-3). No PBT-assessment is included in the REACH registration for the substance; however, based on read-across the registrant has assessed the substance to be readily biodegradable.

5.2 Potential for endocrine disrupting properties

15 of the 28 phthalates were screened not to be bioavailable (Lipinski) indicating a low potential for being biological active (e.g. to have endocrine disrupting properties). Eight of the 28 phthalates were screened to be bioavailable (Lipinski), and thus to have a potential for being biological active. By use of the OECD Toolbox, six of these eight phthalates were screened to form - among several metabolites - monoesters. The monoester metabolised from DEHP has been identified to cause the endocrine disrupting properties for DEHP. Using OECD QSAR Toolbox, none of these eight phthalates was found to be estrogenic receptor (ER) binding, which may cause a subsequent endocrine disruption.

The Lipinski bioavailability was not calculated for five phthalates due to lack of structural information.

5.3 Emission characteristics

Figure 6 shows the distribution of the ERCS for the registered substances with respect to lifecycle stage and with respect to use in opened/closed systems. The figure distinguishes between the phthalates and their alternatives.

It is seen that most of the substances are registered as being manufactured within EU, to be formulated into a mixture/matrix and to have an industrial end-use. In addition, several of the

substances are registered to have wide dispersive uses. Several of the substances are also incorporated into articles and have been assigned a wide-dispersive service life.

In general, the largest emission fractions are uses characterised as industrial end uses and wide dispersive uses such as professional or consumer uses. Therefore, as the phthalates and their alternatives have been registered for uses characterised as opened/closed industrial end uses and wide dispersive uses, significant releases of the phthalates and their alternatives are expected. The releases from industrial uses are more easily controlled and can more easily be reduced than the wide dispersive uses. A decrease in environmental impact from especially wide dispersive uses, could be obtained by replacing the most hazardous substances by less hazardous substances.

The fraction of non-phthalate alternatives reported to have wide dispersive uses is slightly higher than the fraction of the 28 phthalates reported to have wide dispersive uses.

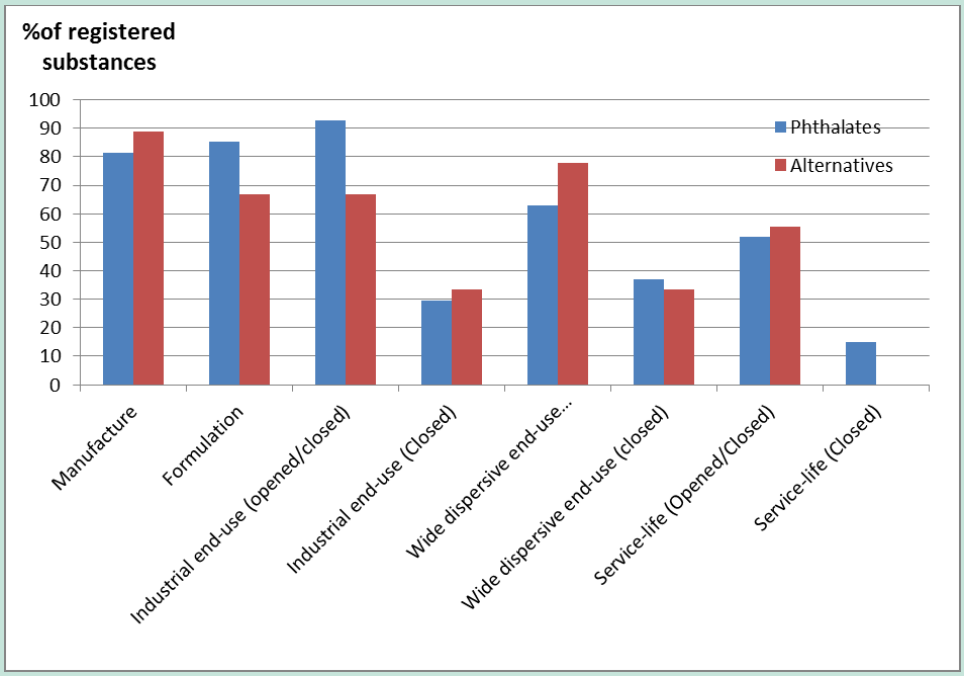

FIGURE 6
DISTRIBUTION OF ERCS ACCORDING TO LIFE-CYCLE AND OPENED/CLOSED CHARACTERISTICS

5.4 Distribution in the environment

The EUSES-calculated regional distributions of the phthalates are shown in Figure 7 and for their identified alternatives in Figure 8. For comparison, the distribution of DEHP is 99% to sediment, 0.97% to soil and less than 0.03% to air and water.

It is seen that none of the phthalates and their alternatives tends to concentrate in water. The distribution to air is of some importance for the short chained phthalates like DEP and DMP, but not for any of the identified alternatives to phthalates. Most of the phthalates and the identified alternatives tend to concentrate to sediment and soil. This is also the case for DEHP.

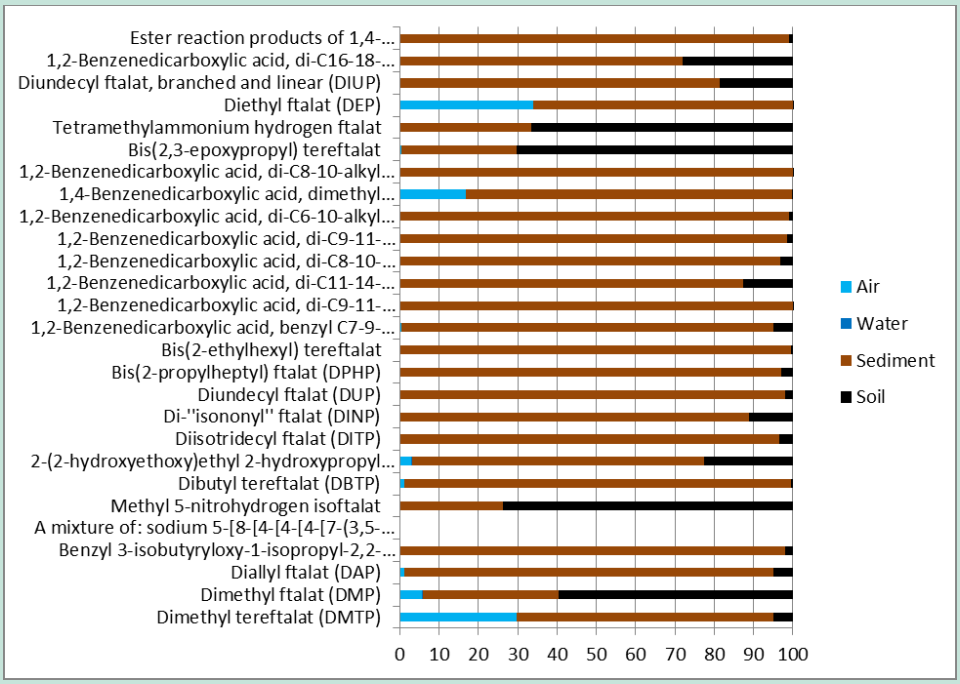

FIGURE 7
EUSES CALCULATED ENVIRONMENTAL DISTRIBUTION OF THE SELECTED PHTHALATES. FOR COMPARISON, THE DISTRIBUTION OF DEHP IS 99% TO SEDIMENT, 0.97% TO SOIL AND LESS THAN 0.03% TO AIR AND WATER.

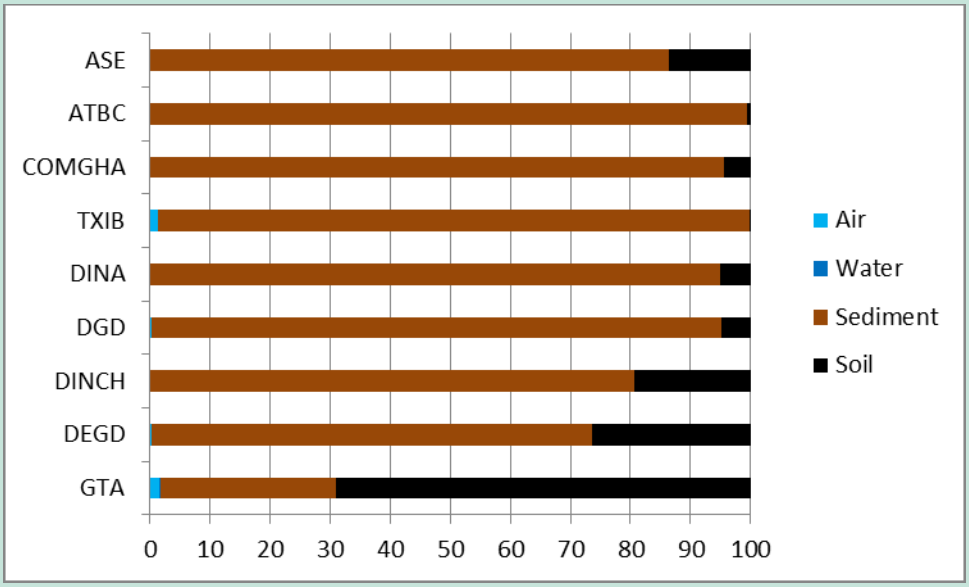

FIGURE 8
EUSES CALCULATED ENVIRONMENTAL DISTRIBUTION OF THE IDENTIFIED ALTERNATIVES TO PHTHALATES

6. Conclusions

Environmental profiles for 28 phthalates and ten alternatives to phthalates (28 substances) have been established. These are reported in separate datasheets. Overall, the water solubility of the phthalates is found to be low and the substances and their alternatives have a high octanol-water partition coefficient increasing almost linearly with the number of carbon. A relation between the octanol-water distribution coefficient (log K_{ow}) and the biodegradability exists. With a few exceptions, phthalates with a log K_{ow} value below approximately 10 are readily biodegradable and phthalates with a log K_{ow} values above 10 are inherently biodegradable. The same overall conclusion is valid for the alternatives to phthalates but the available data set is much smaller and the group of alternative substances does not have the same chemical structure.

There is a general problem with the reported ecotoxicity data, as the reported effect concentrations often exceed the water solubility of the substance tested. This means that the determined toxicities are not necessarily caused by the dissolved substances, but can be a consequence of physical effects. However, from the ecotoxicity data reported with effect concentrations within the water solubility and with an exact value it can be seen that the aquatic toxicity of the phthalates tends to increase with the number of carbon.

None of the registered phthalates and their alternatives is assessed as being a PBT or a vPvB substance. The PBT-profiler indicates that one substance may be a PBT substance. Eight of the 28 phthalates were screened to be bioavailable (Lipinski), and thus to have a potential for being biological active. Six of these eight phthalates may form monoesters, which may have endocrine disrupting properties.

Phthalates and their alternatives have registered opened/closed industrial end uses and wide dispersive uses, and therefore, significant releases of the phthalates and their alternatives into the environment are expected. Especially for the wide dispersive uses, the use of the most hazardous substances should be replaced by less hazardous substances. The fraction of non-phthalate alternatives reported to have wide dispersive uses is slightly higher than the fraction of the 28 phthalates reported to have wide dispersive uses.

It was found that none of the phthalates and their alternatives tends to concentrate in water. The distribution to air is of some importance for the short chained phthalates like DEP and DMP, but not for any of the identified alternatives to phthalates. Most phthalates and identified alternatives tend to concentrate in sediment and soil. This is also the case for DEHP.

When choosing alternatives to e.g. DEHP, alternatives with better or equal environment profiles should be considered and these are represented by phthalates with a carbon number below 20. In addition, a good dataset of equal or better data quality than for DEHP should be ensured for the alternative and the sediment and soil PNEC values for the alternative should be higher than or comparable to the PNEC values for DEHP.

References

[1] Registration dossier (Exp Key)
[2] Registration dossier (Calc Key)
[3] Registration dossier (Exp. Supporting)
[4] Registration dossier (Calc Supporting)
[5] Registration dossier (Calc WoE)
[6] Registration dossier (QSAR WoE)
[7] Registration dossier (Read across subs Key)
[8] Registration dossier (QSAR Key)
[9] Registration dossier (Other Key)
[10] Registration dossier (Read across cat Key)
[11] Registration dossier (Read across subs WoE)
[12] Registration dossier (Exp WoE)
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[14] UNEP (2002): SIDS Initial Assessment Report For SIAM 15: Triacetin.
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[17] ECOSAR

Bilag A: Selection of phthalates

TABLE A.1
SUBSTANCES FOUND IN SPIN

CAS No.	Substance name	Year											Relevant consumption level	Already on list	Polymer?	Di-ester	To be included
		2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011					
100-21-0	1,4-benzenedicarboxylic acid	0.1	0.1	0.3	0.2	0.1	0.1	0.2	0.7	0.9	0.1	6	8	No	No			No
103991-32-8	1,2-benzenedicarboxylic acid, mono[1-methyl-2-[(2-methyl-1-oxo-2-propenyl)oxy] ethyl]ester, polymer with butyl 2-methyl-2-propenoate, butyl 2-propenoate and methyl 2-methyl-2-propenoate	0	0	0	0.1	0	0	0	1.4	0	0	0	0.1	No	No	X	-	No
109694-68-0	1,3-benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 2,2-dimethyl-1,3-propanediol and hexanedioic acid		79.4	64.6		31.7	84.8	70.7	139	87.8				Yes	No	X	X	No
117-81-7	1,2-enzenedicarboxylic acid, bis(2-ethylhexyl) ester	0	0	0	0	0	0	0	0	0	0	0	0	No	No		X	No
117-82-8	1,2-benzenedicarboxylic acid, bis(2-methoxyethyl) ester	0.7	0.2	172.1	31.5	64	64	64	64	4.9	58.3	59		Yes	No		X	Yes
117-84-0	1,2-benzenedicarboxylic acid, dioctyl ester	0.4	0.3	1.5	0.8	64	0	0	0	0	4.8	5	4.8	Yes	Yes		X	No
120-61-6	1,4-benzenedicarboxylic acid, dimethyl ester	0	0	0	0	0	0	0	0	0				No	Yes		X	No
121-91-5	1,3-benzenedicarboxylic acid	0	0	0	0	0	0	0	0	-0	0	0	0	No	No			No
131-11-3	1,2-benzenedicarboxylic acid, dimethyl ester	0	0	0	0	0	0	0	0	0	0	0	0	No	Yes		X	No
166412-78-8	1,2-cyclohexane-dicarboxylic acid, diisononyl ester							0.4	0.4	0.4	0.2	0	0.6	No	Yes		X	No
25214-38-4	1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboylic acid and 2,2-dimethyl-1,3-propanediol		4.4	140.3	135.8	59.1	27.1	11.3	28.1	26.1				Yes	No	X	-	No
25950-34-9	1,3-benzenedicarboxylic acid, polymer with 2,2-dimethyl-1,3-propanediol, 2-ethyl-2-(hydroxymethyl)-1,3-propanediol and hexanedioic acid					8.3	15.4	96.5	93.5	38.6				Yes	No	X	-	No

CAS No.	Substance name	Year												Relevant consumption level	Already on list	Polymer?	Di-ester	To be included
		2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011					
26761-40-0	1,2-benzenedicarboxylic acid, diisodecyl ester	47.8	47.8	11.5	24.3	0.8	0	0	0	0	0	0	0	No	No		X	No
2744-50-5	3,9-perylenedicarboxylic acid, bis(2-methyl-propyl) ester								0	0	0	0	0	No	No		X	No
27554-26-3	1,2-benzenedicarboxylic acid, diisooctyl ester	0	0	0										No	No		X	No
27923-68-8	1,3-benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 2,2-dimethyl-1,3-propanediol and 1,2-ethanediol	0	0	0	0	0	0	4.5	4.5	0	0	0	0	No	No	X	-	No
27987-25-3	1,2-benzenedicarboxylic acid, bis(methylcyclo-hexyl) ester	0.3	0.2	0.2	0.2									No	Yes		X	No
28553-12-0	1,2-benzenedicarboxylic acid, diisononyl ester	6	0.6	0.6	0.2	0.7	0.1	0	0	0	0	0	0.1	No	Yes		X	No
32313-05-6	Bicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid, 1,4,5,6,7,7-hexa-chloro-, polymer with 2,2-bis(hydroxymethyl)-1,3-propanediol and 1,3-isobenzofurandione				28.9	31	31		94.8	45.9	0.3			No	No	X	-	No
32762-75-7	1,3-benzenedicarboxylic acid, polymer with 2,2-dimethyl-1,3-pro-panediol, 2,5-furandione and 1,2-propanediol					31	41							?	No	X	-	No
35176-78-4	1,3-benzenedicarboxylic acid, polymer with dimethyl 1,4-benzene-dicarboxylate, 2,2-di-methyl-1,3-propanediol and 1,2-ethanediol	0	0											No	Yes	X	-	No
35561-07-0	1,3-benzenedicarboxylic acid, polymer with 2,2-dimethyl-1,3-propanediol, 2-ethyl-2-(hydroxymethyl)-1,3-propanediol, hexane-dioic acid and 1,3-isobenzofurandione						1.7	1.1	1.1	0.7	0.7	0		No	No	X	-	No
35636-63-6	1,4-benzenedicarboxylic acid, 2-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azo]-, dimethyl ester					0	0	0	0	0	0	0	1.6	No	No		X	No

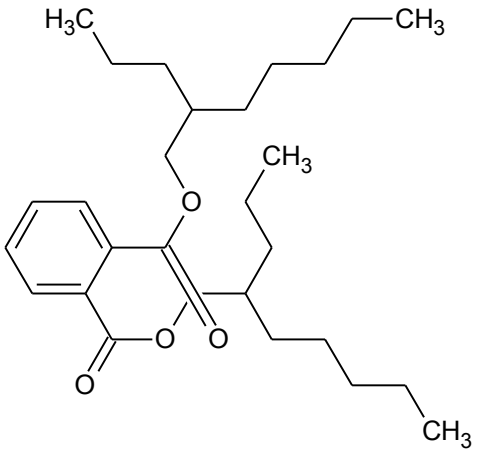
CAS No.	Substance name	Year												Relevant consumption level	Already on list	Polymer?	Di-ester	To be included
		2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011					
40471-09-8	1,3-benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 2,2-dimethyl-1,3-propanediol, 1,2-ethanediol and hexane-dioic acid		10.5	55.1	46.8		9.5							?	No	X	-	No
42847-45-0	1,4-benzenedicarboxylic acid, polymer with 2,2-dimethyl-1,3-propanediol, 1,2-ethanediol, 2-ethyl-2-(hydroxymethyl)-1,3-propanediol and hexane-dioic acid			46										?	No	X	-	No
52247-59-3	1,3-benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 2,2-dimethyl-1,3-propanediol, 2-ethyl-2-(hydroxymethyl)-1,3-propanediol and hexanedioic acid		31.2	97.2		62.6	30.6							?	No	X	-	No
53808-41-6	1,3-benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 2,2-dimethyl-1,3-propanediol and 2-ethyl-2-(hydroxymethyl)-1,3-propanediol		23.4	81.8	55.3	55.6	69.8							?	No	X	-	No
60580-61-2	1,3-benzenedicarboxylic acid, 5-nitro-, zinc salt (1:1)	0	0	0	0	0	0	0	0	0	0	0	0	No	No		-	No
68400-06-6	1,3-benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 2,2-dimethyl-1,3-propanediol and 1,6-hexanediol				53.7	45.1	50.2	72.5	72.5	41.1	36.1			Yes	No	X	-	No
68515-40-2	1,2-benzenedicarboxylic acid, benzyl C7-9-alkyl esters, branched and linear esters					0	0.8	0.6	64.5	0.2	0.1	-1	0	No	Yes		X	No
68515-42-4	1,2-benzenedicarboxylic acid, di-C7-11-alkyl esters, branched and linear			0		0	0							No	No		X	No
68515-43-5	1,2-benzenedicarboxylic acid, di-C9-11-alkyl esters, branched and linear					14.3	18.1	8.6	201	1.6	-0	0	0.2	No	Yes		X	No
68515-48-0	1,2-benzenedicarboxylic acid, di-C8-10-alkyl esters, branched	2	0.7	0.7	0.7		0.1	0	0	0.1	0	0		No	Yes		X	No

CAS No.	Substance name	Year											Relevant consumption level	Already on list	Polymer?	Di-ester	To be included
		2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011					
68515-49-1	1,2-benzenedicarboxylic acid, di-C9-11-alkyl esters, branched	0	0	0	0	1.8	1.2	0.6	0	0	0	0	0	No	Yes		X	No
68515-51-5	1,2-benzenedicarboxylic acid, di-C6-10-alkyl esters	0.9	0.9	0.9	0.6	0	0.2	0.1	0.1	0	0	0		No	Yes		X	No
71662-46-9	1,2-benzenedicarboxylic acid, di-C8-10-alkyl esters	0	0	0.5	0.3	0.6	0.6				0	0	0	No	Yes		X	No
7195-44-0	1,4-benzenedicarboxylic acid, bis(oxiranylmethyl) ester			5.7	5.5		3.2	2.9						No	Yes		X	No
72259-84-8	1,3-benzenedicarboxylic acid, polymer with 2-ethyl-2-(hydroxy-methyl)-1,3-propanediol, hexanedioic acid, 1,6-hexanediol and 1,3-iso-benzofurandione	0.1	2.6	1.5	0.1	0	0	0	0.3	0	0	0	0.2	No	No	X	-	No
84-61-7	1,2-benzenedicarboxylic acid, dicyclohexyl ester	1.1	0.5	0.5	0.4	0	0.1	0.1	0.1	0	0	0	0	No	No		X	No
84-66-2	1,2-benzenedicarboxylic acid, diethyl ester	0	0	0	0	0	0	0	0	0	0	0	0	No	Yes		X	No
84-69-5	1,2-benzenedicarboxylic acid, bis(2-methyl-propyl) ester	0.4	0	0	0.1	0.1	0.2	0	0	0	0	0	0	No	No		X	No
84-74-2	1,2-benzenedicarboxylic acid, dibutyl ester	0	0	0	0	0	0	0	0	0	0	0	0	No	No		X	No
84-77-5	1,2-benzenedicarboxylic acid, didecyl ester	1.3	1.3	1.3	0.8									No	No		X	No
85507-79-5	1,2-benzenedicarboxylic acid, diundecyl ester, branched and linear						47.3	16.1	20.5	19.2	9.5	6	11.6	Yes	Yes		X	No
85-68-7	1,2-benzenedicarboxylic acid, butyl phenylmethyl ester	0.1	0.1	0.1	-0	0	0	-0	-0	-0	-1	0	0	No	No		X	No
88-99-3	1,2-benzenedicarboxylic acid	0	0	0	0	0	0	0	0	0	0	0		No	No			No
89-08-7	1,2-benzenedicarboxylic acid, 4-sulfo-												0.1	No	No			No
90144-49-3	1,3-benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 2,2-dimethyl-1,3-propanediol, 1,2-ethanediol, 2-ethyl-2-(hydroxymethyl)-1,3-propanediol and hexane-dioic acid		9.7					97.2	97.8	72.1				Yes	No	X	-	No

CAS No.	Substance name	Year											Relevant consumption level	Already on list	Polymer?	Di-ester	To be included
		2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011					
9065-68-3	1,3-benzenedicarboxylic acid, polymer with 2,5-furandione, oxybis[propanol] and 1,2-propanediol			42.4	18.3	1.1	43.9	48.6	48.6					Yes	No	X	-	No
93762-48-2	1,2-benzenedicarboxylic acid, nonyl ester, branched and linear	152.4	152.4											Yes	No			No

1,2-benzenedicarboxylic acid, benzyl C7-9-branched and linear alkyl esters

Identification of substance

CAS No.	68515-40-2
EINECS No.	271-082-5
IUPAC name	-
Structure	
SMILES	O=C(OCC(CCCCC)CCC)c(c(ccc1)C(=O)OCC(CCCCC)CCC)c1

REACH

Registration	Full
Submission	Joint submission
Total tonnage	10,000 - 100,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (53); Aquatic Acute 1 H400 (28)
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	446.68 g/mole	
Vapour pressure	0.000117 Pa, 25°C (Modified Grain method, MPBPVPWIN) Klimisch score: 2	[8]
Henry's law constant	-	
Water solubility	0.00979 mg/L, 25°C, pH 7 (WSKOWWIN v1.41) Klimisch score: 2	[8]
Log K_{OW}	6.66, 20 °C, pH 7 (KOWWIN v1.67a) Klimisch score: 2	[8]

Ecotoxicological data

Algae	EC50 (*Selenastrum capricornutum*, 96 hours): > 1000 ppm* (OECD Guideline 201) (Read-across) Klimisch score: 2	[7]
Crustaceans	LC50 (*Daphnia magna*, 48 hours): 4.5 mg/L* (American Public Health Association. 1975. Standard Methods for the Examination of Water and Wastewater. 14th ed., New York) Klimisch score: 2	[1]
	NOEC (-): 0.039 mg/L (-) Klimisch score: -	[15]
Fish	LC50 (*Oncorhynchus mykiss*, 96 hours): >1000 mg/L* (USEPA (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975) Klimisch score: 2	[1]
	MATC (*Pimephales promelas*, 30 days): 0.3 mg/L (-) Klimisch score: -	[15]
Terrestrial plants	-	
Soil macroorganisms	-	
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	-	

Environmental fate

Bioconcentration factor (BCF)	156 - 886 (OECD Guideline 305 E) Klimisch score: 2	[1]
Ready biodegradability	Readily biodegradable (OECD Guideline 301 B) (read-across) Klimisch score: 2	[7]
Adsorption/desorption	log K_{OC}: 3.974 (KOCWIN v2.00) Klimisch score: 2	[8]

PBT

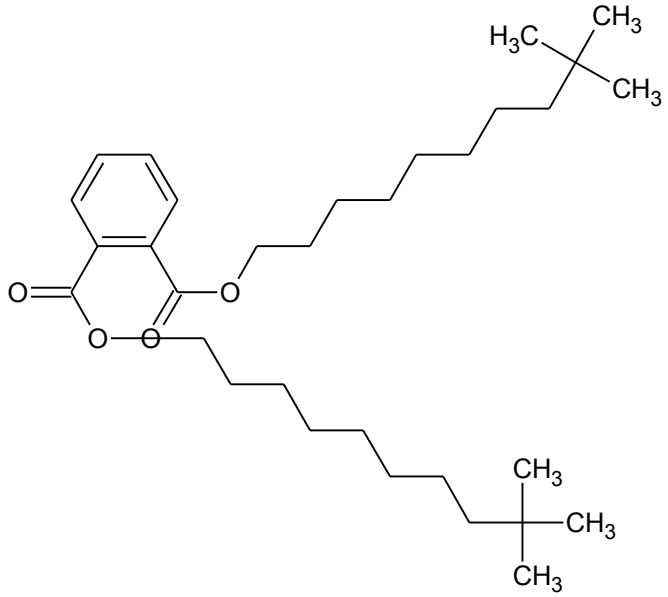
REACH registration dossier	-
QSAR	P: Neg; B: Neg; T: Pos; BCF: 3.2 Fish ChV (mg/L): 2.5 Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 2.3

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	219 metabolites formed. Of these: 209 bioavailable and 10 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	22 metabolites formed. Of these: 22 bioavailable and 0 not-bioavailable. Monoesters formed.
Skin metabolism	33 metabolites formed. Of these: 29 bioavailable and 4 not-bioavailable. Monoesters formed.

1,2-benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13-rich

Identification of substance

CAS No.	68515-47-9
EINECS No.	271-089-3
IUPAC name	-
Structure	
SMILES	O=C(c1ccccc1C(=O)OCCCCCCCCCC(C)(C)C)OCCCCCCCCCC(C)(C)C

REACH

Registration	Full
Submission	Joint submission
Total tonnage	1,000-10,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (85)
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	Yes
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	502.78 g/mole	
Vapour pressure	0.000000000363 hPa, 25°C (QSPR quantitative structure-property relationship) Klimisch score: 2	[9]
Henry's law constant	275 Pa m³/mol, 25°C (QSPR quantitative structure-property relationship) Klimisch score: 2	[2]
Water solubility	0.00007 µg/L, 25°C, pH 7 (SPR Quantitative structure-property relationship) Klimisch score: 2	[2]
Log Kow	12.06, 25°C, pH 7 (mathematical model) Klimisch score: 2	[9]

Ecotoxicological data

Algae	EC50 (*Selenastrum capricornutum*, 8 days): >0.6 mg/L* (USEPA 600/9-78-018, Printz Algal Assay Bottle Test. 1978) Klimisch score: 1	[1]
Crustaceans	LC50 (*Daphnia magna*, 48 hours): >0.05 mg/L* (USEPA, 660/3-75-009 Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975) Klimisch score: 1	[1]
	NOEC (*Daphnia magna*, 21 days): 0.052 mg/L* (US EPA Environmental Effects Test Guidelines, ES-1, EPA 560/6-82-002) Klimisch score: 1	[1]
Fish	LC50 (*Oncorhynchus mykiss*, 96 hours): >0.15 mg/L* (USEPA, 660/3-75-009 Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians) Klimisch score: 1	[1]
	NOEC (*Oncorhynchus mykiss*, 120 days): 0.3 mg/L* (US Environmental Protection Agency, Toxic Substance Control Act EPA-TSCA 40 CFR, Part 797.1600) (Read-across) Klimisch score: 1	[7]
Terrestrial plants	L[E]C50 (*Triticum aestivum; Brassica alba; Lepidum sativum*, 17 days): >100 mg/kg soil dw (OECD Guideline 208) Klimisch score: 2	[7]
Soil macroorganisms	LC50 (*Eisenia fetida*, 14 days): >7664 mg/kg (OECD Guideline 207) (Read-across) Klimisch score: 1	[7]
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	-	

Environmental fate

Bioconcentration factor (BCF)	1 L/kg (no guideline followed) Klimisch score: 2	[1]
Ready biodegradability	Inherently biodegradable, not fulfilling specific criteria (OECD Guideline 301 F) Klimisch score: 1	[1]
Adsorption/desorption	log K_{OC}: 6.08 EPA OTS 796.2750 (Sediment and Soil Adsorption Isotherm) Klimisch score: 2	[1]

PBT

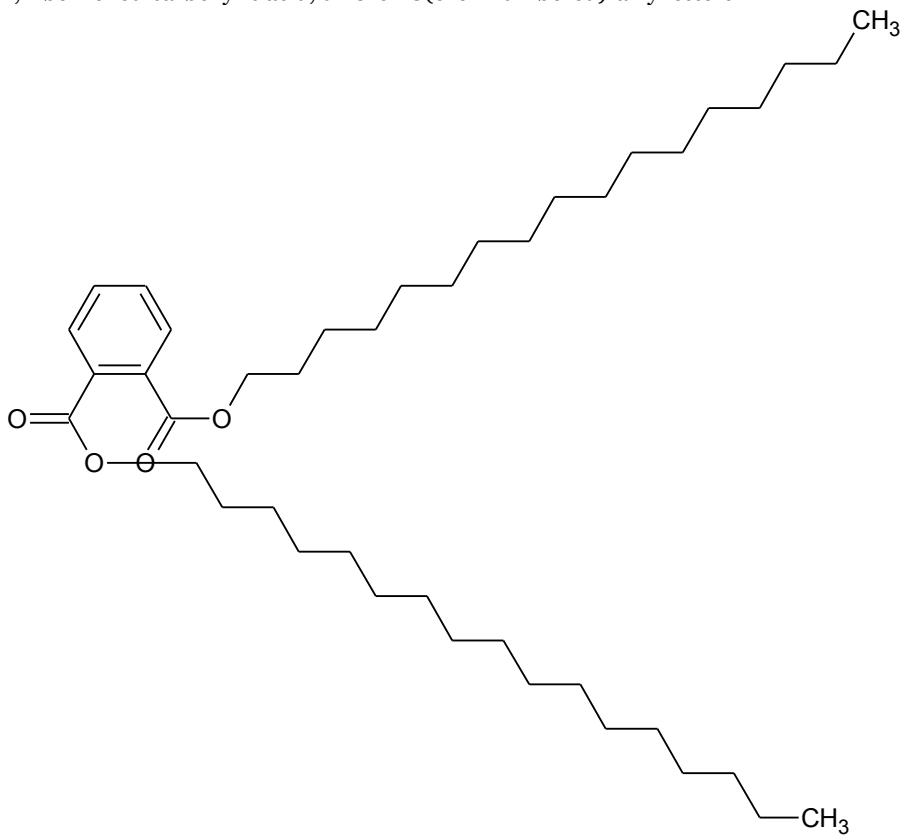
REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Pos; B: Neg; T: ??; BCF: 36 Fish ChV (mg/L): ?? Half-life (Water, days): 60 Half-life (Soil, days): 120 Half-life (Sediment, days): 540 Half-life (Air, days): 0.67

QSAR bioavailability

Lipinski	n.d.
Mammalian metabolism	
Microbial metabolism (observed)	
Microbial metabolism (simulated)	
Rat In vivo metabolism (observed)	
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	
Rat Liver S9 metabolism (simulated)	
Skin metabolism	

1,2-benzenedicarboxylic acid, di-C16-18-alkyl esters

Identification of substance

CAS No.	90193-76-3
EINECS No.	290-580-3
IUPAC name	1,2-benzenedicarboxylic acid, di-C16-18(even numbered)-alkyl esters
Structure	
SMILES	O=C(c1ccccc1C(=O)OCCCCCCCCCCCCCCCCCC)OCCCCCCCCCCCCCCCCCC

REACH

Registration	Full
Submission	Joint submission
Total tonnage	1,000 - 10,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (18)
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	643.06 g/mole	
Vapour pressure	1.61xE-20 Pa, 20°C (Calculation based on SPARC online calculator http://ibmlc2.chem.uga.edu/sparc/, University of Georgia, USA) Klimisch score: 2	[8]
Henry's law constant	-	
Water solubility	<0.05 mg/L, 20°C, pH 6.84 (EU Method A.6 (Water Solubility)) Klimisch score: 1	[1]
Log K_{OW}	17.38 (KOWWIN v1.67) Klimisch score: 2	[8]

Ecotoxicological data

Algae	EL50 (*Pseudokirchnerella subcapitata*, 72 hours): >100% (OECD Guideline 201) Klimisch score: 1	[1]
Crustaceans	EC0 (*Daphnia magna*, 48 hours): >= 10,000 mg/L* (DIN 38412/11) (Read-across) Klimisch score: 2 -	[7]
Fish	LC50 (*Oncorhynchus mykiss*, 96 hours): >100 mg/L* (OECD Guideline 203) (Read-across) Klimisch score: 2 -	[7]
Terrestrial plants	-	
Soil macroorganisms	-	
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	-	

Environmental fate

Bioconcentration factor (BCF)	3.162 L/kg (BCFBAF v3.00) Klimisch score: 2	[4]
Ready biodegradability	Not readily biodegradable (OECD Guideline 301 B) Klimisch score: 1	[1]
Adsorption/desorption	log K_{OC}: 10.4 (KOCWIN v2.00) Klimisch score: 2	[2]

PBT

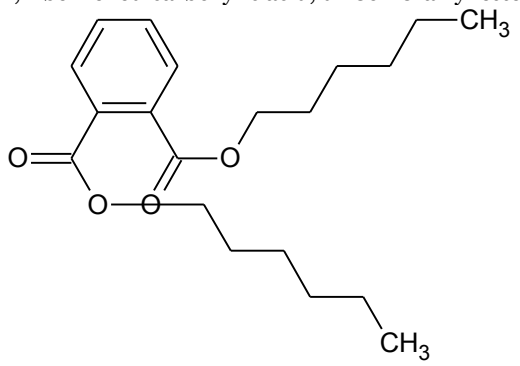
REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Pos; B: Neg; T: ??; BCF: 3.2 Fish ChV (mg/L): ?? Half-life (Water, days): 38 Half-life (Soil, days): 75 Half-life (Sediment, days): 340 Half-life (Air, days): 0.35

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	187 metabolites formed. Of these: 96 bioavailable and 91 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	7 metabolites formed. Of these: 0 bioavailable and 7 not-bioavailable. Monoesters formed.
Skin metabolism	n.d.

1,2-benzenedicarboxylic acid, di-C6-10-alkyl esters

Identification of substance

CAS No.	68515-51-5
EINECS No.	271-094-0
IUPAC name	1,2-benzenedicarboxylic acid, di-C6-10-alkyl esters
Structure	
SMILES	O=C(c1ccccc1C(=O)OCCCCCC)OCCCCCC

REACH

Registration	Full
Submission	Joint Submission
Total tonnage	100 - 1,000 tonnes per annum
Harmonised classification	
Notified classification	Not Classified (2)
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	Yes
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	Yes

Physico-chemical characteristics

Molecular weight	334.46 g/mole	
Vapour pressure	<0.001 mBar, 38°C (ASTM D 2879) Klimisch score: 2	[1]
Henry's law constant	0.901 Pa m³/mol, 25°C (EPIWIN (v 4.0), HENRYWIN Program (v 3.20)) Klimisch score: 2	[2]
Water solubility	11 mg/L, 23°C, pH 5.5 (ASTM E 1148) Klimisch score: 2	[1]
Log K_{OW}	8.2, 20°C, pH 7 (ASTM E 1147) Klimisch score: 2	[1]

Ecotoxicological data

Algae	EC50 (*Scenedesmus subspicatus*, 72 hours): >2.8 mg/L (EU Method C.3 (Algal Inhibition test)) (Read-across) Klimisch score: 2	[1]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): >1.7 mg/L (EU Method C.2 (Acute Toxicity for Daphnia)) Klimisch score: 2	[1]
	NOEC (*Daphnia magna*, 21 days): 0.059 mg/L (no guideline followed) (Read-across) Klimisch score: 2	[7]
Fish	LC50 (*Brachydanio rerio*, 96 hours): >0.32 mg/L (EU Method C.1 (Acute Toxicity for Fish)) (Read-across) Klimisch score: 2	[7]
	NOEC (*Oncorhynchus mykiss*, 155 days): 0.3 mg/L (EPA OPPTS 850.1400 (Fish Early-life Stage Toxicity Test)) Klimisch score: 2	[7]
Terrestrial plants	LC50 (*Triticum aestivum; Brassica alba; Lepidum sativum*, 18 days): > 100 mg/kg soil dw (OECD guideline 208) Klimisch score: 2	[1]
Soil macroorganisms	LC10 (*Eisenia fetida*, 14 days): >1000 mg/kg soil dw (EU Method C.8 (Toxicity for Earthworms: Artificial Soil Test)) Klimisch score: 2	[1]
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	-	

Environmental fate

Bioconcentration factor (BCF)	1,033 L/kg (EPIWIN (v 4.1), BCFBAF (v3.01)) Klimisch score: 2	[2]
Ready biodegradability	readily biodegradable (EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test)) Klimisch score: 2	[1]
Adsorption/desorption	log K_{OC} (first main component): 5.55, 20.1°C; log K_{OC} (second component): 7.6, 20.1°C (OECD Guideline 121) Klimisch score: 2	[1]

PBT

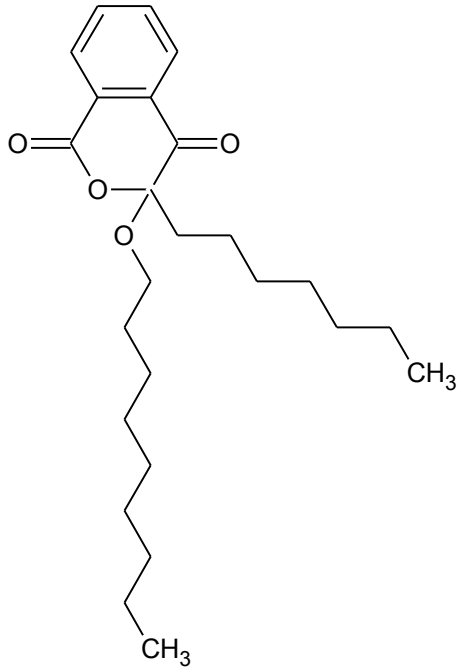
REACH registration dossier	-
QSAR	P: Neg; B: Neg; T: Pos; BCF: 620 Fish ChV (mg/L): 0.003 Half-life (Water, days): 8.7 Half-life (Soil, days): 17 Half-life (Sediment, days): 78 Half-life (Air, days): 1.1

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	45 metabolites formed. Of these: 40 bioavailable and 5 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	5 metabolites formed. Of these: 5 bioavailable and 0 not-bioavailable. Monoesters formed.
Skin metabolism	8 metabolites formed. Of these: 6 bioavailable and 2 not-bioavailable. Monoesters formed.

1,2-benzenedicarboxylic acid, di-C8-10-alkyl esters

Identification of substance

CAS No.	71662-46-9
EINECS No.	275-809-7
IUPAC name	1,2-benzenedicarboxylic acid, di-C8-10-alkyl esters
Structure	
SMILES	CCCCCCCCCOC(=O)c1ccccc1C(=O)OCCCCCCCC

REACH

Registration	Full
Submission	Joint submission
Total tonnage	1,000-10,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (51)
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	404.6 g/mole	
Vapour pressure	< 0.001 mBar, 38°C (ASTM D 2879) (Read-across) Klimisch score: 2	[7]
Henry's law constant	1.01 Pa m³/mol, 25 C (EPIWIN (v 4.0), HENRYWIN Program (v 3.20)) Klimisch score: 2	[2]
Water solubility	ca. 0.00005572 mg/L, 25°C (Water Solubility Estimate from log K_{OW} (WSKOW v1.42)) Klimisch score: 2	[2]
Log K_{OW}	8.2, 20°C, pH ca. 7 (ASTM E 1147) (Read-across) Klimisch score: 2	[7]

Ecotoxicological data

Algae	EC50 (*Scenedesmus subspicatus*, 72 hours): >0.83 mg/L* (EU Method C.3 (Algal Inhibition test)) Klimisch score: 2	[1]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): >4.3 mg/L* (EU Method C.2 (Acute Toxicity for Daphnia)) Klimisch score: 2	[1]
	NOEC (*Daphnia magna*, 21 days): 0.059 mg/L* (no guideline followed) (read-across) Klimisch score: 2	[7]
Fish	LC50 (*Brachydanio rerio*, 96 hours): >0.32 mg/L* (EU Method C.1 (Acute Toxicity for Fish)) Klimisch score: 2	[1]
	NOEC (*Oncorhynchus mykiss*, 155 days): 0.3 mg/L* (EPA OPPTS 850.1400 (Fish Early-life Stage Toxicity Test)) (Read-across) Klimisch score: 2	[7]
Terrestrial plants	L[E]50 (Triticum aestivum; Brassica alba; Lepidum sativum, 19 days): >100 mg/kg soil dw (OECD guideline 208) Klimisch score: 2	[1]
Soil macroorganisms	LC10 (*Eisenia fetida*, 14 days): >1000 mg/kg soil dw (EU Method C.8 (Toxicity for Earthworms: Artificial Soil Test)) Klimisch score: 2	[1]
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	-	

Environmental fate

Bioconcentration factor (BCF)	341 L/kg (BCFBAF (v3.00)) Klimisch score: 2	[2]
Ready biodegradability	Readily biodegradable (EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test)) Klimisch score: 2	[1]
Adsorption/desorption	log K_{OC}: 5.409 (KOCWIN (v2.00), MCI method) Klimisch score: 2	[2]

PBT

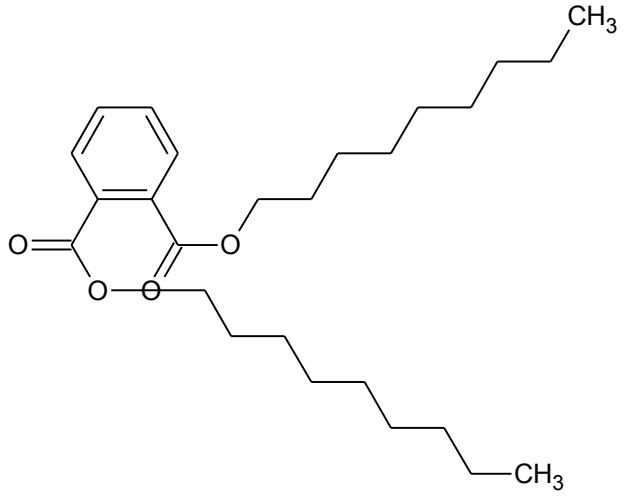
REACH registration dossier	
QSAR	P: Neg; B: Neg; T: ??; BCF: 340 Fish ChV (mg/L): ?? Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 0.75

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	88 metabolites formed. Of these: 61 bioavailable and 27 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	9 metabolites formed. Of these: 8 bioavailable and 1 not-bioavailable. Monoesters formed.
Skin metabolism	16 metabolites formed. Of these: 11 bioavailable and 5 not-bioavailable. Monoesters formed.

1,2-benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich

Identification of substance

CAS No.	68515-48-0
EINECS No.	271-090-9
IUPAC name	-
Structure	
SMILES	O=C(c1ccccc1C(=O)OCCCCCCCCCC)OCCCCCCCCCC

REACH

Registration	Full
Submission	Joint submission
Total tonnage	100,000-1,000,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (243). 3 notifiers with Repr. 2 H361
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	Yes
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	418.62 g/mole	
Vapour pressure	Approx. 0.00006 Pa, 20°C (calculation) Klimisch score: 2	[2]
Henry's law constant	41.4 Pa m³/mol, 25°C (Henry's Law constant is calculated based on vapour pressure and water solubility) Klimisch score: 2	[2]
Water solubility	0.6 µg/L, 21°C, pH 7 (equivalent or similar to OECD Guideline 105) Klimisch score: 2	[1]
Log Kow	8.8, 25°C, pH 7 (OECD Guideline 123) Klimisch score: 2	[1]

Ecotoxicological data

Algae	EC50 (*Selenastrum capricornutum*, 5 days): >1.8 mg/L* (USEPA 600/9-78-018, Printz Algal Assay Bottle Test) Klimisch score: 1	[1]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): >0.06 mg/L* (USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians) Klimisch score: 1	[1]
	NOEC (*Daphnia magna*, 21 days): 0.0036 mg/L* (OECD Guideline 211) Klimisch score: 1	[1]
Fish	LC50 (*Cyprinodon variegatus*, 96 hours): >0.52 mg/L* (USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians) Klimisch score: 1	[1]
	NOEC (*Oryzias latipes*, 284 days): >= 18.5 <= 24.5 other: ug/g feed (OECD Guideline 210) Klimisch score: 2	[1]
Terrestrial plants	NOEC (*Lactuca sativa*, 5 days): 1018 g/kg artificial soil (d.w.) (U.S. EPA-600/3-88/029 Protocols for Short Term Toxicity Screening of Hazardous Waste Sites (NTIS / PB88-235510/AS)) Klimisch score: 1	[1]
Soil macroorganisms	LC50 (*Eisenia fetida*, 14 days): >7270 mg/kg natural soil d (OECD Guideline 207) Klimisch score: 1	[1]
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	30 mg/kg soil dw (Assessment factor: 50)	

Environmental fate

Bioconcentration factor (BCF)	<3 L/kg (no guideline followed) Klimisch score: 2	[1]
Ready biodegradability	Readily biodegradable (OECD Guideline 301 F) Klimisch score: 2	[1]
Adsorption/desorption	log K_{OC}: 5.9 (PCKOCWIN version 2.00) Klimisch score: 2	[2]

PBT

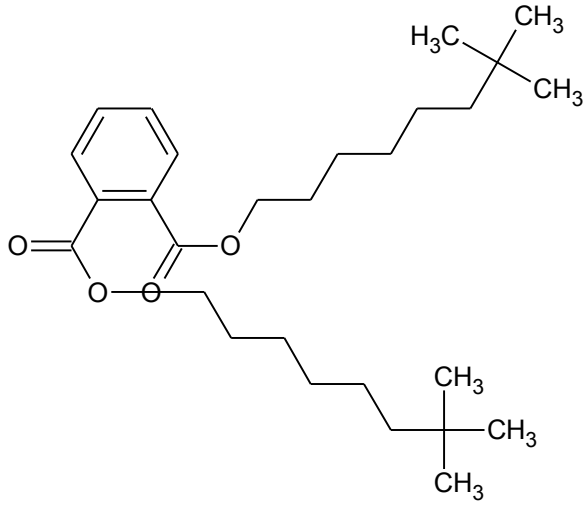
REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Neg; B: Neg; T: ??; BCF: 200 Fish ChV (mg/L): ?? Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 0.67

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	170 metabolites formed. Of these: 142 bioavailable and 28 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	2 metabolites formed. Of these: 1 bioavailable and 1 not-bioavailable. Monoesters formed.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	16 metabolites formed. Of these: 12 bioavailable and 4 not-bioavailable. Monoesters formed.
Skin metabolism	36 metabolites formed. Of these: 23 bioavailable and 13 not-bioavailable. Monoesters formed.

1,2-benzenedicarboxylic acid, di-C9-11-branched alkyl esters, C10-rich

Identification of substance

CAS No.	68515-49-1
EINECS No.	271-091-4
IUPAC name	-
Structure	
SMILES	O=C(c1ccccc1C(=O)OCCCCCCCC(C)(C)C)OCCCCCCCC(C)(C)C

REACH

Registration	Full
Submission	Joint submission
Total tonnage	100,000-1,000,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (382). No classification for reproduction toxicity
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	Yes
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	446.68 g/mole	
Vapour pressure	0.000051 Pa, 25°C (regression using Clausius-clapeyron equation) Klimisch score: 2	[2]
Henry's law constant	114 Pa m³/mol, 25°C (Henry's Law constant is calculated based on vapor pressure and water solubility) Klimisch score: 2	[2]
Water solubility	0.00017 mg/L, 21°C, pH 7 (OECD Guideline 105) Klimisch score: 2	[1]
Log Kow	8.8, 25°C, pH 7 (OECD Guideline 123) Klimisch score: 2	[1]

Ecotoxicological data

Algae	EC50 (*Selenastrum capricornutum*, 8 days): >0.8 mg/L* (USEPA 600/9-78-018, Printz Algal Assay Bottle Test) Klimisch score: 1	[1]
Crustaceans	LC50 (*Daphnia magna*, 48 hours): >0.02 mg/L* (USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians) Klimisch score: 1	[1]
	NOEC (*Daphnia magna*, 21 days): 0.0034 mg/L* (OECD Guideline 211) Klimisch score: 1	[1]
Fish	LC50 (*Oncorhynchus mykiss*, 96 hours): >0.62 mg/L* (USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians) Klimisch score: 1	[1]
	NOEC (*Oryzias latipes*, 284 days): >= 19.2 <= 22.7 other: ug/g feed (OECD Guideline 210) Klimisch score: 2	[1]
Terrestrial plants	EC50 (*Lolium species*, 5 days): 8551 mg/kg artificial soil (d.w.) (U.S. EPA-600/3-88/029 Protocols for Short Term Toxicity Screening of Hazardous Waste Sites (NTIS / PB88-235510/AS)) Klimisch score: 1	[1]
Soil macroorganisms	LC50 (*Eisenia fetida*, 14 days): >7664 mg/kg natural soil dw (OECD Guideline 207) Klimisch score: 1	[1]
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	-	

Environmental fate

Bioconcentration factor (BCF)	<1 L/kg (Study report; company data) Klimisch score: 2	[1]
Ready biodegradability	Readily biodegradable, but failing 10-day window (OECD Guideline 301 F) Klimisch score: 2	[1]
Adsorption/desorption	log K_{OC}: 5.46 (EPA OTS 796.2750 (Sediment and Soil Adsorption Isotherm)) Klimisch score: 2	[1]

PBT

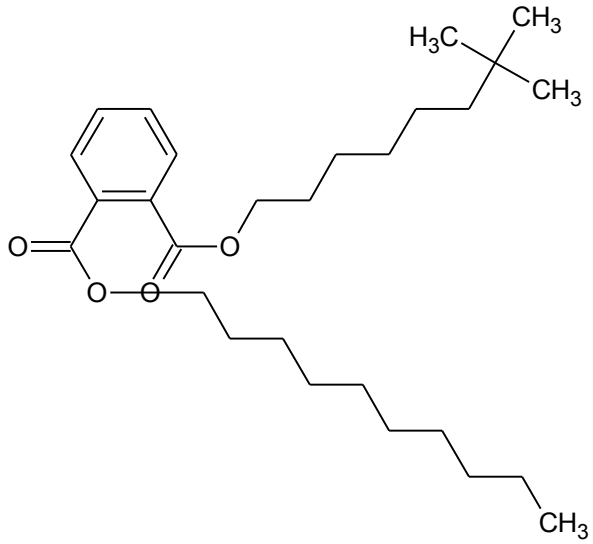
REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Pos; B: Neg; T: ??; BCF: 83 Fish ChV (mg/L): ?? Half-life (Water, days): 60 Half-life (Soil, days): 120 Half-life (Sediment, days): 540 Half-life (Air, days): 0.83

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	132 metabolites formed. Of these: 120 bioavailable and 12 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	11 metabolites formed. Of these: 8 bioavailable and 3 not-bioavailable. Monoesters formed.
Skin metabolism	34 metabolites formed. Of these: 22 bioavailable and 12 not-bioavailable. Monoesters formed.

1,2-benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters

Identification of substance

CAS No.	68515-43-5
EINECS No.	271-085-1
IUPAC name	1,2-benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters
Structure	
SMILES	O=C(c1ccccc1C(=O)OCCCCCCCCCC)OCCCCCCC(C)(C)C

REACH

Registration	Full
Submission	Joint submission
Total tonnage	1,000-10,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (99); Acute Tox. 2 H300 (1)
Wide dispersive end use opened/closed	No
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	446.68 g/mole	
Vapour pressure	0.000357 hPa, 25°C (EPIWIN v 4.0, MPBVP v1.43) Klimisch score: 2	[2]
Henry's law constant	3.72 Pa m³/mol, 25°C (EPIWIN v 4.0, HENRYWIN Program v 3.20) Klimisch score: 2	[2]
Water solubility	0.9385 µg/L, 25°C (EPIWIN v 4.0, WSKOW v1.41) Klimisch score: 2	[2]
Log Kow	8.3, 55°C, pH 7.3 (OECD Guideline 117) Klimisch score: 1	[1]

Ecotoxicological data

Algae	EC50 (*Scenedesmus subspicatus*, 72 hours): >0.83 mg/L* (EU Method C.3 Algal Inhibition test) (Read-across) Klimisch score: 2	[7]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): > 4.3 mg/L* (EU Method C.2 Acute Toxicity for Daphnia) Klimisch score: 2	[7]
	NOEC (*Daphnia magna*, 21 days): 0.56 mg/L* (OECD Guideline 202 1984) Klimisch score: 2	[1]
Fish	LC50 (*Brachydanio rerio*, 96 hour): >0.32 mg/L* (EU Method C.1 Acute Toxicity for Fish) (Read-across) Klimisch score: 2	[7]
	NOEC (*Oncorhynchus mykiss*, 155 days): 0.3 mg/L* (EPA OPPTS 850.1400 Fish Early-life Stage Toxicity Test) (Read-across) Klimisch score: 1	[7]
Terrestrial plants	L[E]C50 (*Triticum aestivum; Brassica alba; Lepidum sativum*, 19 days): > 100 mg/kg soil dw (OECD guideline 208) (Read-across) Klimisch score: 2	[7]
Soil macroorganisms	LC10 (*Eisenia fetida*, 14 days): >1000 mg/kg soil dw (EU Method C.8 Toxicity for Earthworms: Artificial Soil Test) (Read-across) Klimisch score: 2	[7]
PNEC (fresh water)	5.6 µg/L (Assessment factor: 10)	
PNEC (marine water	0.56 µg/L (Assessment factor: 100)	
PNEC (fresh water sediment)	11.4 mg/kg sediment dw	
PNEC (marine water sediment)	1.14 mg/kg sediment dw	
PNEC (soil)	1 mg/kg soil dw (Assessment factor: 1000)	

Environmental fate

Bioconcentration factor (BCF)	2339 L/kg wet weight (BCFBAF v3.00) Klimisch score: 2	[2]
Ready biodegradability	Readily biodegradable (EU Method C.4-C Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test; OECD Guideline 301 B) Klimisch score: 1	[1]
Adsorption/desorption	log K_{OC}: 5.3849 (KOCWIN v2.00) Klimisch score: 2	[2]

PBT

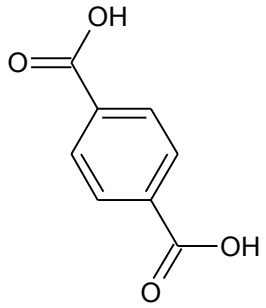
REACH registration dossier	-
QSAR	P: Pos; B: Neg; T: ??; BCF: 73 Fish ChV (mg/L): ?? Half-life (Water, days): 38 Half-life (Soil, days): 75 Half-life (Sediment, days): 340 Half-life (Air, days): 0.71

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	166 metabolites formed. Of these: 128 bioavailable and 38 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	9 metabolites formed. Of these: 9 bioavailable and 0 not-bioavailable. Monoesters formed.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	3 metabolites formed. Of these: 3 bioavailable and 0 not-bioavailable. Monoesters formed.
Rat Liver S9 metabolism (simulated)	14 metabolites formed. Of these: 12 bioavailable and 2 not-bioavailable. Monoesters formed.
Skin metabolism	26 metabolites formed. Of these: 20 bioavailable and 6 not-bioavailable. Monoesters formed.

1,4-benzenedicarboxylic acid, dimethyl ester, manuf. of, by-products from

Identification of substance

CAS No.	68988-22-7
EINECS No.	273-521-6
IUPAC name	1,4-benzenedicarboxylic acid, dimethyl ester, manuf. of, by-products from
Structure	
SMILES	O=C(O)C1=CC=C(C(O)=O)C=C1

REACH

Registration	Full
Submission	Joint submission
Total tonnage	10,000-100,000 tonnes per annum
Harmonised classification	
Notified classification	Skin Sens. 1 H317 Aquatic Chronic 3 H412 (3)
Wide dispersive end use opened/closed	No
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	166.13 g/mole	
Vapour pressure	0.536 Pa, 20°C (OECD Guideline 104) Klimisch score: 1	[1]
Henry's law constant	-	
Water solubility	< 0.983 mg/L, 20°C, pH 7.2 (visual observation) Klimisch score: 2	[1]
Log Kow	3.2, 25°C, pH 2 and pH 7 (OECD Guideline 117) Klimisch score: 1	[1]

Ecotoxicological data

Algae	EC50 (*Pseudokirchnerella subcapitata*, 72 hours): 3.2 mg/L* (OECD Guideline 201) Klimisch score: 1	[1]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): 3.9 mg/L* (OECD Guideline 202) Klimisch score: 1	[1]
	-	
Fish	EC50 (*Cyprinus carpio*, 96 hours): >1.4 mg/L* (OECD Guideline 203) Klimisch score: 1	[1]
	-	
Terrestrial plants	-	
Soil macroorganisms	-	
PNEC (fresh water)	32 µg/L (Assessment factor: 1000)	
PNEC (marine water	3.2 µg/L (Assessment factor: 10000)	
PNEC (fresh water sediment)	1.29 mg/kg sediment dw	
PNEC (marine water sediment)	0.13 mg/kg sediment dw	
PNEC (soil)	0.24 mg/kg soil dw (Assessment factor: -)	

Environmental fate

Bioconcentration factor (BCF)	-	
Ready biodegradability	Not readily biodegradable (OECD Guideline 301 B) Klimisch score: 1	[1]
Adsorption/desorption	log K_{OC}: 1.624 - 2.962 (KOCWIN Vers. 2.00) (Read-across) (WOE) Klimisch score: 4	[11]

PBT

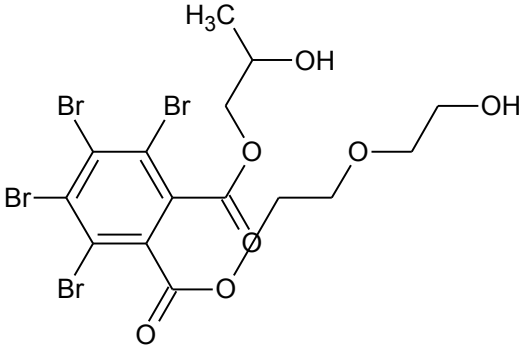
REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: -; B: -; T: -; BCF: - Fish ChV (mg/L): - Half-life (Water, days): - Half-life (Soil, days): - Half-life (Sediment, days): - Half-life (Air, days): -

QSAR bioavailability

Lipinski	Bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	2 metabolites formed. Of these: 2 bioavailable and 0 not-bioavailable. Monoesters formed.
Microbial metabolism (simulated)	11 metabolites formed. Of these: 11 bioavailable and 0 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	n.d.
Skin metabolism	n.d.

2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl 3,4,5,6-tetrabromophthalate

Identification of substance

CAS No.	20566-35-2
EINECS No.	243-885-0
IUPAC name	2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl 3,4,5,6-tetrabromophthalate
Structure	
SMILES	O=C(OCCOCCO)c(c(c(c(c1Br)Br)Br)C(=O)OCC(O)C)c1Br

REACH

Registration	Full
Submission	Joint submission
Total tonnage	100-1,000 tonnes per annum
Harmonised classification	
Notified classification	Aquatic Chronic 3 H412 (71); Not classified (23)
Wide dispersive end use opened/closed	No
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	627.91 g/mole	
Vapour pressure	2.37E-14 mm Hg (MPBPBP) Klimisch score: 2	[2]
Henry's law constant	2.23E-021 atm-m3/mole (EPI Suite v3.20) Klimisch score: 1	[2]
Water solubility	0.05697 mg/L, 25 °C (WSKOW) Klimisch score: 2	[2]
Log K_{OW}	3.8256 (KOWWIN) Klimisch score: 2	[2]

Ecotoxicological data

Algae	EC50 (-, 96 hours): 0.849 mg/L* (EPI Suite v3.20) Klimisch score: 2	[2]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): 10.779 mg/L* (EPI Suite v3.20) Klimisch score: 2	[2]
	-	
Fish	LC50 (*Lepomis macrochirus*, 96 hours): 12 mg/L* (Ecological Research Series EPA-660/3-75-009, April, 1975. 61 pp) Klimisch score: 2	[1]
	LC50 (-, 30 days): 1.116 mg/L* ((EPI) Suite™ v3.2) Klimisch score: 2	[2]
Terrestrial plants	-	
Soil macroorganisms	-	
PNEC (fresh water)	0.011 mg/L (Assessment factor: 100)	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	-	

Environmental fate

Bioconcentration factor (BCF)	39 (BCF v2.17) Klimisch score: 2	[2]
Ready biodegradability	The reference substance is not expected to be readily biodegradable (EPIwin) Klimisch score: 2	[2]
Adsorption/desorption	K_{OC}: 10 (PCKOCWIN v1.66) Klimisch score: 2	[2]

PBT

REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Pos; B: Neg; T: Pos; BCF: 86 Fish ChV (mg/L): 0.37 Half-life (Water, days): 60 Half-life (Soil, days): 120 Half-life (Sediment, days): 540 Half-life (Air, days): 0.54

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	116 metabolites formed. Of these: 78 bioavailable and 38 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	17 metabolites formed. Of these: 8 bioavailable and 9 not-bioavailable. Monoesters formed.
Skin metabolism	6 metabolites formed. Of these: 4 bioavailable and 2 not-bioavailable. Monoesters formed.

A mixture of: sodium 5-[8-[4-[4-[4-[7-(3,5-dicarboxylatophenylazo)-8-hydroxy-3,6-disulfonatonaphthalen-1-ylamino]-6-hydroxy-1,3,5-triazin-2-yl]-2,5-dimethylpiperazin-1-yl]-6-hydroxy-1,3,5-triazin-2-ylamino]-1-hydroxy-3,6-disulfonatonaphthalen-2-ylazo]-isophthalate; ammonium 5-[8-[4-[4-[4-[7-(3,5-dicarboxylatophenylazo)-8-hydroxy-3,6-disulfonatonaphthalen-1-ylamino]-6-hydroxy-1,3,5-triazin-2-yl]-2,5-dimethylpiperazin-1-yl]-6-hydroxy-1,3,5-triazin-2-ylamino]-1-hydroxy-3,6-disulfonatonaphthalen-2-ylazo]-isophthalate; 5-[8-[4-[4-[4-[7-(3,5-dicarboxylatophenylazo)-8-hydroxy-3,6-disulfonatonaphthalen-1-ylamino]-6-hydroxy-1,3,5-triazin-2-yl]-2,5-dimethylpiperazin-1-yl]-6-hydroxy-1,3,5-triazin-2-ylamino]-1-hydroxy-3,6-disulfonaphthalen-2-ylazo]-isophthalic acid

Identification of substance

CAS No.	187285-15-0
EINECS No.	413-180-4
IUPAC name	-
Structure	N/A
SMILES	-

REACH

Registration	NONS
Submission	Individual submission
Total tonnage	Tonnage data confidential
Harmonised classification	Eye dam 1; H318
Notified classification	-
Wide dispersive end use opened/closed	No
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	g/mole
Vapour pressure	-
	Klimisch score:
Henry's law constant	-
Water solubility	-
	Klimisch score:
Log K_{OW}	-
	Klimisch score:

Ecotoxicological data

Algae	-
	-
Crustaceans	-
	-
Fish	-
	-
Terrestrial plants	-
Soil macroorganisms	-
PNEC (fresh water)	-
PNEC (marine water	-
PNEC (fresh water sediment)	-
PNEC (marine water sediment)	-
PNEC (soil)	-

Environmental fate

Bioconcentration factor (BCF)	-
Ready biodegradability	-
Adsorption/desorption	-

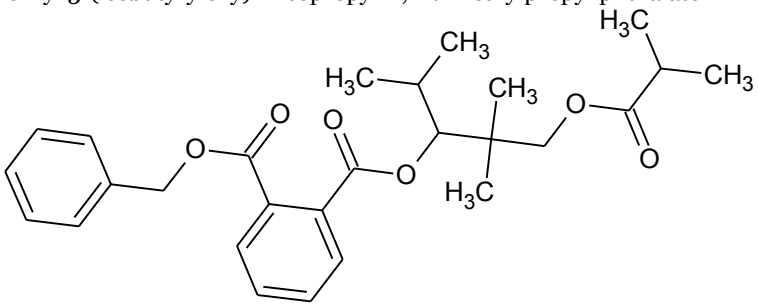
PBT

REACH registration dossier	-
QSAR	P: -; B: -; T: -; BCF: -
	Fish ChV (mg/L): -
	Half-life (Water, days): -
	Half-life (Soil, days): -
	Half-life (Sediment, days): -
	Half-life (Air, days): -

QSAR bioavailability	
Lipinski	n.d.
Mammalian metabolism	
Microbial metabolism (observed)	
Microbial metabolism (simulated)	
Rat In vivo metabolism (observed)	
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	
Rat Liver S9 metabolism (simulated)	
Skin metabolism	

Benzyl 3-isobutyryloxy-1-isopropyl-2,2-dimethylpropyl phthalate

Identification of substance

CAS No.	16883-83-3
EINECS No.	240-920-1
IUPAC name	Benzyl 3-(isobutyryloxy)-1-isopropyl-2,2-dimethylpropyl phthalate
Structure	
SMILES	O=C(OCC(C)(C)C(OC(=O)c(c(ccc1)C(=O)OCc(cccc2)c2)c1)C(C)C)C(C)C

REACH

Registration	Full
Submission	Joint submission
Total tonnage	1,000-10,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (76); Acute Tox. 4 H302 Aquatic Chronic 1 H410 (3)
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	454.57 g/mole	
Vapour pressure	0.000000848 Pa, 25°C (MPBPVPWIN v1.43, modified Grain method) Klimisch score: 2	[8]
Henry's law constant	-	
Water solubility	0.00147 mg/L, 25°C, pH 7 (WSKOWWIN v1.41) Klimisch score: 2	[8]
Log K_{OW}	7, 20°C, pH 7 (KOWWIN v1.67a) Klimisch score: 2	[8]

Ecotoxicological data

Algae	EC50 (*Pseudokirchnerella subcapitata*, 96 hours): >1,000 ppm* (OECD Guideline 201) Klimisch score: 2	[1]
Crustaceans	LC50 (*Daphnia magna*, 48 hours): >7.5 mg/L* (American Public Health Association. 1975. Standard Methods for the Examination of Water and Wastewater. 14th ed., New York) Klimisch score: 2	[1]
	-	
Fish	LC50 (*Oncorhynchus mykiss*, 96 hours): >1000 mg/L* (OECD Guideline 203) Klimisch score: 2	[1]
	-	
Terrestrial plants	-	
Soil macroorganisms	-	
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	-	

Environmental fate

Bioconcentration factor (BCF)	155-886 (OECD Guideline 305 E) Klimisch score: 2	[1]
Ready biodegradability	Readily biodegradable (OECD Guideline 301 B) (Read-across) Klimisch score: 2	[7]
Adsorption/desorption	log K_{OC}: 4.666 (KOCWIN v2.00) Klimisch score: 2	[8]

PBT

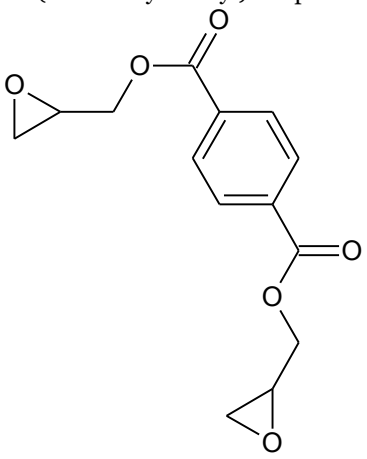
REACH registration dossier	-
QSAR	P: Pos; B: Pos; T: Pos; BCF: 13000 Fish ChV (mg/L): 0.0019 Half-life (Water, days): 38 Half-life (Soil, days): 75 Half-life (Sediment, days): 340 Half-life (Air, days): 0.92

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	98 metabolites formed. Of these: 78 bioavailable and 20 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	16 metabolites formed. Of these: 13 bioavailable and 3 not-bioavailable. Monoesters formed.
Skin metabolism	6 metabolites formed. Of these: 4 bioavailable and 2 not-bioavailable. Monoesters formed.

Bis(2,3-epoxypropyl) terephthalate

Identification of substance

CAS No.	7195-44-0
EINECS No.	230-565-0
IUPAC name	Bis(oxiran-2-ylmethyl) terephthalate
Structure	
SMILES	O1C(COC(=O)c2ccc(C(=O)OCC3OC3)cc2)C1

REACH

Registration	Full
Submission	Joint submission
Total tonnage	100-1,000 tonnes per annum
Harmonised classification	
Notified classification	Skin Irrit. 2 H315 Skin Sens. 1 H317 Eye Irrit. 2 H319 Aquatic Chronic 2 H411 (250); Skin Irrit. 2 H315 Skin Sens. 1 H317 Eye Irrit. 2 H319 Aquatic Chronic 2 H411 (47); Skin Irrit. 2 H315 Skin Sens. 1 H317 Eye Irrit. 2 H319 STOT SE 3 H335 Aquatic Chronic
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	278.26 g/mole	
Vapour pressure	<= 0.0000678 Pa, 20°C (OECD Guideline 104) Klimisch score: 1	[1]
Henry's law constant	-	
Water solubility	77 mg/L, 20°C, pH ca. 5 (OECD Guideline 105) Klimisch score: 1	[1]
Log Kow	1.7, 25°C (OECD Guideline 117) Klimisch score: 1	[1]

Ecotoxicological data

Algae	EC50 (*Pseudokirchnerella subcapitata*, 72 hours): 1.13 mg/L NOEC (Pseudokirchnerella subcapitata, 72 hours,): 0.327 mg/L (OECD Guideline 201) Klimisch score: 1	[1]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): 81 mg/L* (EU Method C.2 (Acute Toxicity for Daphnia)) Klimisch score: 2 -	[1]
Fish	LC50 (*Cyprinus carpio*, 96 hours): 8.8 mg/L (EU Method C.1 (Acute Toxicity for Fish)) Klimisch score: 2 -	[1]
Terrestrial plants	-	
Soil macroorganisms	-	
PNEC (fresh water)	0.00294 mg/L (Assessment factor: 1000)	
PNEC (marine water	0.000294 mg/L (Assessment factor: 10000)	
PNEC (fresh water sediment)	0.00869 mg/kg sediment dw	
PNEC (marine water sediment)	0.000869 mg/kg sediment dw	
PNEC (soil)	0.00553 mg/kg soil dw	

Environmental fate

Bioconcentration factor (BCF)	-	
Ready biodegradability	Readily biodegradable (OECD Guideline 301 F) Klimisch score: 1	[1]
Adsorption/desorption	log K_{OC}: 2, 25 °C (OECD Guideline 121) Klimisch score: 1	[1]

PBT

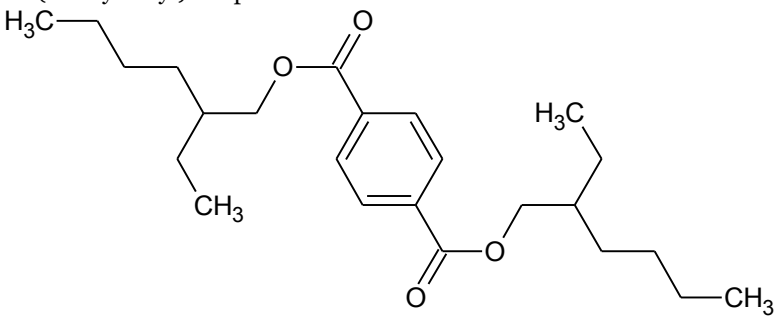
REACH registration dossier	-
QSAR	P: Neg; B: Neg; T: Pos; BCF: 3.2 Fish ChV (mg/L): 0.55 Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 3.3

QSAR bioavailability

Lipinski	Bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	33 metabolites formed. Of these: 32 bioavailable and 1 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	2 metabolites formed. Of these: 2 bioavailable and 0 not-bioavailable. Monoesters formed.
Skin metabolism	6 metabolites formed. Of these: 6 bioavailable and 0 not-bioavailable. Monoesters formed.

Bis(2-ethylhexyl) terephthalate

Identification of substance

CAS No.	6422-86-2
EINECS No.	229-176-9
IUPAC name	Bis(2-ethylhexyl) terephthalate
Structure	
SMILES	O=C(OCC(CCCC)CC)c(ccc(c1)C(=O)OCC(CCCC)CC)c1

REACH

Registration	Full
Submission	Joint submission
Total tonnage	10,000-100,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (166); No classification for reproduction toxicity
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	Yes
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	390.57 g/mole	
Vapour pressure	<0.001 Pa, 25°C (EU Method A.4 (Vapour Pressure)) Klimisch score: 2	[1]
Henry's law constant	-	
Water solubility	Approx. 0.4 µg/L, 22.5°C, pH ca. 5 (Method Reference: Ellington, JJ, 1999, J. Chem. Eng. Data, 44, 1414-1418) Klimisch score: 2	[1]
Log K_{OW}	7.81, 25°C, pH 7 (QSAR (SPARC) used and acceptable in accordance with REACH Annex XI) (WOE) Klimisch score: 2	[6]

Ecotoxicological data

Algae	EC50 (*Selenastrum capricornutum*, 72 hours): >0.86 mg/L* (OECD Guideline 201) Klimisch score: 1	[1]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): >1.4 µg/L* (OECD Guideline 202) Klimisch score: 1	[1]
	NOEC (*Daphnia magna*, 21 days): >= 0.76 µg/L* (OECD Guideline 211) Klimisch score: 1	[1]
Fish	LC50 (*Pimephales promelas*, 96 hours): >984 mg/L* (OECD Guideline 203) Klimisch score: 2	[1]
	NOEC (*Oncorhynchus mykiss*, 60 days): >=0.28 mg/L* (ASTM. 1983. Proposed New Standard Practice for Conducting Fish Early Life Stages Toxicity Tests. Draft No. 7.) Klimisch score: 1	[1]
Terrestrial plants	EC50 (*Lolium perenne*, 14 days): >1,400 µg/L (SEPA. 1982. Early Seedling Growth Toxicity Test, EG-13) Klimisch score: 1	[1]
Soil macroorganisms	-	
PNEC (fresh water)	0.08 µg/L (Assessment factor: 10)	
PNEC (marine water	0.008 µg/L (Assessment factor: 100)	
PNEC (fresh water sediment)	8.28 mg/kg sediment dw (AF: 100)	
PNEC (marine water sediment)	0.828 mg/kg sediment dw (AF: 1000)	
PNEC (soil)	15 µg/kg soil dw (Assessment factor: 1000)	

Environmental fate

Bioconcentration factor (BCF)	393 (EPA OPPTS 850.1710 (Oyster Bioconcentration Test)) Klimisch score: 1	[1]
Ready biodegradability	Readily biodegradable (OECD Guideline 301 B) Klimisch score: 1	[1]
Adsorption/desorption	log K_{OC}: 5.43, 25°C (QSAR EPIWIN-KOWIN) (WOE) Klimisch score: 2	[6]

PBT

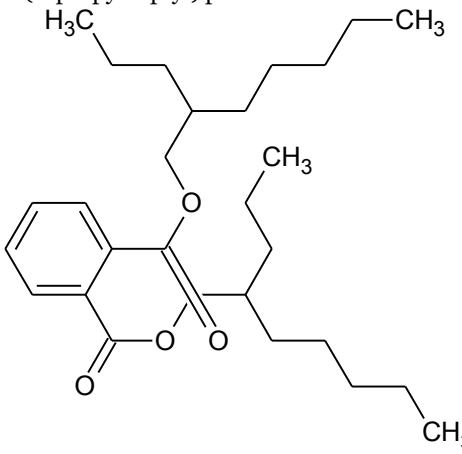
REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Neg; B: Neg; T: ??; BCF: 700 Fish ChV (mg/L): ?? Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 0.75

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	60 metabolites formed. Of these: 46 bioavailable and 14 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	5 metabolites formed. Of these: 4 bioavailable and 1 not-bioavailable. Monoesters formed.
Skin metabolism	14 metabolites formed. Of these: 9 bioavailable and 5 not-bioavailable. Monoesters formed.

Bis(2-propylheptyl) phthalate (DPHP)

Identification of substance

CAS No.	53306-54-0
EINECS No.	258-469-4
IUPAC name	Bis(2-propylheptyl) phthalate
Structure	
SMILES	O=C(OCC(CCCCC)CCC)c(c(ccc1)C(=O)OCC(CCCCC)CCC)c1

REACH

Registration	Full
Submission	Joint submission
Total tonnage	100,000-1,000,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (133)
Wide dispersive end use opened/closed	No
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	446.68 g/mole	
Vapour pressure	0.000000037 hPa, 20°C (EU Method A.4 Vapour Pressure) Klimisch score: 1	[1]
Henry's law constant	3.72 Pa m³/mol, 25°C (EpiWin calculation) Klimisch score: 2	[4]
Water solubility	<0.0001 mg/L, 25°C (EU Method A.6 Water Solubility) Klimisch score: 1	[1]
Log Kow	>6, 25°C, pH 5.77 (EU Method A.8 Partition Coefficient) Klimisch score: 1	[1]

Ecotoxicological data

Algae	EC50 (*Scenedesmus subspicatus*, 72 hours): >100 mg/L* (EU Method C.3 Algal Inhibition test) Klimisch score: 1	[1]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): >100 mg/L* (EU Method C.2 Acute Toxicity for Daphnia) Klimisch score: 1	[1]
	NOEC (*Daphnia magna*, 21 days): >1 mg/L* (OECD Guideline 211) Klimisch score: 2	[1]
Fish	LC50 (*Brachydanio rerio*, 96 hours): >10000 mg/L* (OECD Guideline 203) Klimisch score: 1	[1]
	-	
Terrestrial plants	-	
Soil macroorganisms	-	
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	-	

Environmental fate

Bioconcentration factor (BCF)	<14.4 (OECD Guideline 305 C) (Read-across) Klimisch score: 2	[7]
Ready biodegradability	Readily biodegradable (OECD Guideline 301 B) Klimisch score: 1	[1]
Adsorption/desorption	log K_{OC}: >5.63 (OECD Guideline 121) Klimisch score: 1	[1]

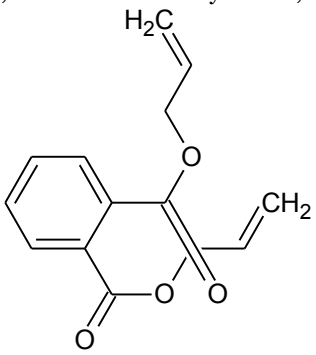
PBT

REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Neg; B: Neg; T: ??; BCF: 76 Fish ChV (mg/L): ?? Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 0.58

QSAR bioavailability	
Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	81 metabolites formed. Of these: 53 bioavailable and 28 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	5 metabolites formed. Of these: 4 bioavailable and 1 not-bioavailable. Monoesters formed.
Skin metabolism	14 metabolites formed. Of these: 9 bioavailable and 5 not-bioavailable. Monoesters formed.

Diallyl phthalate (DAP)

Identification of substance

CAS No.	131-17-9
EINECS No.	205-016-3
IUPAC name	1,2-benzenedicarboxylic acid, di-2-propenyl ester
Structure	
SMILES	O=C(OCC=C)c(c(ccc1)C(=O)OCC=C)c1

REACH

Registration	Full
Submission	Joint submission
Total tonnage	100-1,000 tonnes per annum
Harmonised classification	Acute tox 4; H302 Aquatic acute 1; H400 Aquatic chronic 1; H410
Notified classification	
Wide dispersive end use opened/closed	No
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	246.26 g/mole	
Vapour pressure	0.15 Pa, 25°C (Estimation Program Interface (EPI) Suite. Ver.3.12. Nov 30, 2004) (WOE) Klimisch score: 2	[5]
Henry's law constant	0.039 Pa m³/mol, 25°C (no guideline followed) Klimisch score: 4	[3]
Water solubility	0.148 g/L, 20°C (OECD Guideline 105) Klimisch score: 1	[1]
Log K_{OW}	3.23, 20°C (OECD Guideline 107) Klimisch score: 2	[1]

Ecotoxicological data

Algae	EC50 (*Scenedesmus subspicatus*, 72 hours): 3.8 mg/L (DIN 38412, Part 9) Klimisch score: 2	
Crustaceans	EC50 (*Daphnia magna*, 48 hours): 5.5 mg/L (OECD Guideline 202) Klimisch score: 1	[1]
	NOEC (*Daphnia magna*, 21 days): 3.2 mg/L (Provisionnal Procedure: extended toxicology test with Daphnia magna (determination of NOEC for reproduction rate, mortality and the time of the first appearance of offspring; 21 d)) Klimisch score: 2	[1]
Fish	LC50 (*Oncorhynchus mykiss*, 96 hours): 0.24 mg/L (OECD Guideline 203) Klimisch score: 1	[1]
	-	
Terrestrial plants	-	
Soil macroorganisms	-	
PNEC (fresh water)	2.3 µg/L (Assessment factor: 100)	
PNEC (marine water	23 ng/L (Assessment factor: 1000)	
PNEC (fresh water sediment)	0.154 ng/kg sediment dw	
PNEC (marine water sediment)	0.002 ng/kg sediment dw	
PNEC (soil)	1.77 µg/kg soil dw	

Environmental fate

Bioconcentration factor (BCF)	61 (Bioconcentration Factor was determined with (Q)SAR) (WOE) Klimisch score: 4	[5]
Ready biodegradability	Inherent, ultimate biodegradable (OECD Guideline 302 C) Klimisch score: 2	[1]
Adsorption/desorption	K_{OC}: 429 (EPISUITE calculation of K_{OC}) (WOE) Klimisch score: 2	[6]

PBT

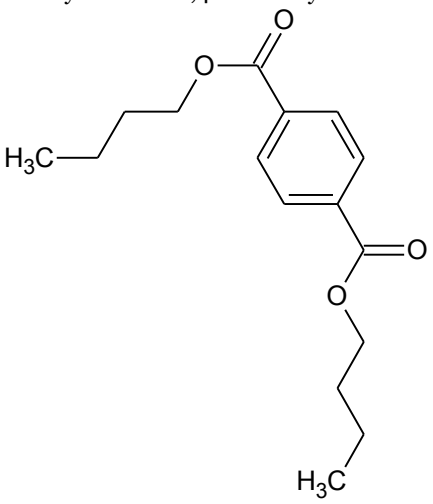
REACH registration dossier	-
QSAR	P: Neg; B: Neg; T: Pos; BCF: 63 Fish ChV (mg/L): 0.014 Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 0.18

QSAR bioavailability

Lipinski	Bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	38 metabolites formed. Of these: 38 bioavailable and 0 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	4 metabolites formed. Of these: 3 bioavailable and 1 not-bioavailable. Monoesters formed.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	5 metabolites formed. Of these: 5 bioavailable and 0 not-bioavailable. Monoesters formed.
Skin metabolism	2 metabolites formed. Of these: 2 bioavailable and 0 not-bioavailable. Monoesters formed.

Dibutyl terephthalate (DBTP)

Identification of substance

CAS No.	1962-75-0
EINECS No.	217-803-9
IUPAC name	Dibutylbenzene-1,4 dicarboxylate
Structure	
SMILES	CCCCOC(=O)c1ccc(cc1)C(=O)OCCCC

REACH

Registration	Full
Submission	Joint submission
Total tonnage	100-1,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (12)
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	Yes
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	278.35 g/mole	
Vapour pressure	<0.038 Pa, 25°C (EU Method A.4 (Vapour Pressure)) Klimisch score: 2	[1]
Henry's law constant	-	
Water solubility	0.00451 mg/L, 24°C (OECD Guideline 105) Klimisch score: 1	[1]
Log K_{OW}	4.74, 25°C, påH 7 (QSAR (SPARC software) used for estimation, in accordance with REACH Annex XI.) (WOE) Klimisch score: 2	[6]

Ecotoxicological data

Algae	EC50 (*Pseudokirchnerella subcapitata*, 72 hours): >0.013 mg/L* (OECD Guideline 201) Klimisch score: 1	[1]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): >0.34 mg/L* (OECD Guideline 202) Klimisch score: 1	[1]
	NOEC (*Daphnia magna*, 21 days): >=50 µg/L* (OECD Guideline 211) Klimisch score: 1	[1]
Fish	LC50 (*Pimephales promelas*, 96 hours): >0.17 mg/L* (OECD Guideline 203) Klimisch score: 1	[1]
	NOEC (*Pimephales promelas*, 32 days): >=24 µg/L* (OECD Guideline 210) Klimisch score: 1	[1]
Terrestrial plants	-	
Soil macroorganisms	-	
PNEC (fresh water)	1.3 µg/L (Assessment factor: 10)	
PNEC (marine water	0.13 µg/L (Assessment factor: 100)	
PNEC (fresh water sediment)	0.344 mg/kg sediment dw	
PNEC (marine water sediment)	0.0344 mg/kg sediment dw	
PNEC (soil)	0.0682 mg/kg soil dw	

Environmental fate

Bioconcentration factor (BCF)	393 (EPA OPPTS 850.1710 (Oyster Bioconcentration Test)) (Read-across) Klimisch score: 1	[11]
Ready biodegradability	Readily biodegradable (OECD Guideline 301 B) Klimisch score: 1	[1]
Adsorption/desorption	log K_{OC}: 3.85, 25°C (EPISUITE-KOCWIN) (WOE) Klimisch score: 2	[6]

PBT

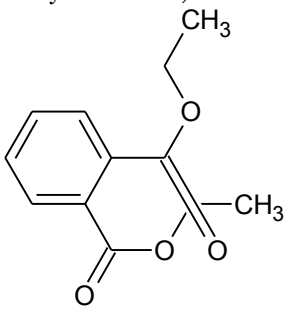
REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Neg; B: Pos; T: Pos; BCF: 2100 Fish ChV (mg/L): 0.048 Half-life (Water, days): 8.7 Half-life (Soil, days): 17 Half-life (Sediment, days): 78 Half-life (Air, days): 1.8

QSAR bioavailability

Lipinski	Bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	n.d.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	n.d.
Skin metabolism	n.d.

Diethyl phthalate (DEP)

Identification of substance

CAS No.	84-66-2
EINECS No.	201-550-6
IUPAC name	Diethyl benzene-1,2-dicarboxylate
Structure	
SMILES	O=C(OCC)c(c(ccc1)C(=O)OCC)c1

REACH

Registration	Full
Submission	Joint submission
Total tonnage	1,000-10,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (1046); 1 out of approx. 1100 claims Repr 2 H361
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	Yes

Physico-chemical characteristics

Molecular weight	222.2372 g/mole	
Vapour pressure	< 28 mBar, 25° (EU Method A.4 (Vapour Pressure)) Klimisch score: 1	[1]
Henry's law constant	0.0399 Pa-m³/mole (HENRYWIN Program (v 3.20)) Klimisch score: 2	[2]
Water solubility	932 mg/L, 20°C, pH 7.2 (EPA OPPTS 830.7840 (Water Solubility)) Klimisch score: 1	[1]
Log Kow	2.2, 41°C, pH 7.5 (OECD Guideline 117) Klimisch score: 1	[1]

Ecotoxicological data

Algae	EC50 (*Scenedesmus subspicatus*, 72 hour): 23 mg/L (DIN 38 412) Klimisch score: 2	[1]
Crustaceans	LC50 (*daphnia*, 48 hour): 90 mg/L (EPA-660/3-75-009) Klimisch score: 2	[1]
	NOEC (*Daphnia magna*, 21 days): 25 mg/L (Internal EG&G Bionomics protocol 1982 & amendment EGG/CMA-008) Klimisch score: 2	[1]
Fish	LC50 (*Oncorhynchus mykiss*, 96 hour): 12 mg/L (EPA-660/3-75-009) Klimisch score: 2	[1]
	LOEC (*Cyprinus carpio*, 28 d): >= 0.1 <= 1 mg/L (-) Klimisch score: -	[16]
Terrestrial plants	LC50 (*growth*, 14 days): 134 mg/kg dry soil (OECD 208) Klimisch score: 2	[1]
Soil macroorganisms	LC50 (*Eisenia fetida*, 48 hours): 0.85 mg/cm² (OECD 207) Klimisch score: 2	[3]
PNEC (fresh water)	12 µg/L (Assessment factor: 1000)	
PNEC (marine water	1.2 µg/L (Assessment factor: 10000)	
PNEC (fresh water sediment)	137 µg/kg sediment dw	
PNEC (marine water sediment)	13.7 µg/kg sediment dw	
PNEC (soil)	137 µg/kg soil dw (Assessment factor: -)	

Environmental fate

Bioconcentration factor (BCF)	13.14 L/kg wet weight (BCFBAF v3.00) Klimisch score: 2	[2]
Ready biodegradability	Readily biodegradable (US EPA 1982, Chemical fate test guidelines EPA560/6-82-003 US environmental protection agency Washington DC USA) Klimisch score: 2	[1]
Adsorption/desorption	log $k_{OC,soil}$: 2.34 (EU Method C.19 (Estimation of the Adsorption Coefficient (KOC) on Soil and Sewage Sludge Using High Performance Liquid Chromatography (HPLC))) Klimisch score: 1	[1]

PBT

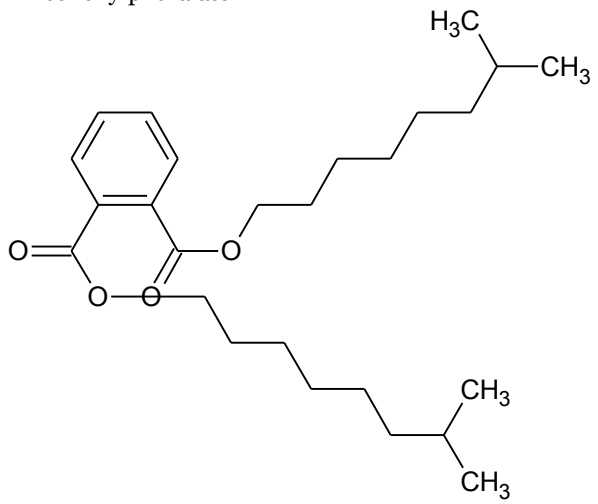
REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Neg; B: Neg; T: Pos; BCF: 18 Fish ChV (mg/L): 0.82 Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 4.6

QSAR bioavailability

Lipinski	Bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	27 metabolites formed. Of these: 27 bioavailable and 0 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	1 metabolites formed. Of these: 1 bioavailable and 0 not-bioavailable. Monoesters formed.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	5 metabolites formed. Of these: 5 bioavailable and 0 not-bioavailable. Monoesters formed.
Skin metabolism	5 metabolites formed. Of these: 5 bioavailable and 0 not-bioavailable. Monoesters formed.

Di-"isononyl" phthalate (DINP)

Identification of substance

CAS No.	28553-12-0
EINECS No.	249-079-5
IUPAC name	Di-isononylphthalate
Structure	
SMILES	O=C(c1ccccc1C(=O)OCCCCCCC(C)C)OCCCCCCC(C)C

REACH

Registration	Full
Submission	Joint submission
Total tonnage	100,000-1,000,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (795); No classification for reproduction toxicity
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	Yes
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	Yes

Physico-chemical characteristics

Molecular weight	418.62 g/mole	
Vapour pressure	0.00006 Pa, 20°C (Several measurements in the 80s and 90s cited in the EU Risk Assessment) Klimisch score: 2	[9]
Henry's law constant	41.4 Pa m³/mol, 25°C (Henry's Law constant is calculated based on vapour pressure and water solubility) Klimisch score: 2	[4]
Water solubility	0.6 µg/L, 21°C, pH 7 (OECD Guideline 105) Klimisch score: 2	[1]
Log K_{OW}	8.8-9.7 (OECD Guideline 117) Klimisch score: 2	[1]

Ecotoxicological data

Algae	EC50 (*esmodesmus subspicatus*, 72 hours): >88 mg/L* (EU Method C.3 Algal Inhibition test) Klimisch score: 1	[1]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): >74 mg/L* (EU Method C.2 Acute Toxicity for Daphnia) Klimisch score: 1	[1]
	NOEC (*Daphnia magna*, 21 days): >101 mg/L* (OECD guideline 202 Part II) Klimisch score: 2	[1]
Fish	LC50 (*Brachydanio rerio*, 96 hours): > 102 mg/L* (EU Method C.1 Acute Toxicity for Fish) Klimisch score: 1	[1]
	NOEC (*Oryzias latipes*, 284 days): >= 18.5 <= 24.5 µg/g feed (OECD Guideline 210 (Fish, Early-Life Stage Toxicity Test) with evaluation of two generations) Klimisch score: 2	[1]
Terrestrial plants	NOEC (*Lepidum sativum; Triticum aestivum; Lactuca sativa*, 22 days): 1000 mg/kg soil dw (OECD Guideline 208) Klimisch score: 1	[1]
Soil macroorganisms	LC50 (*Eisenia fetida*, 14 days): >7270 mg/kg natural soil dw (OECD Guideline 207) Klimisch score: 1	[1]
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	30 mg/kg soil dw (Assessment factor: 50)	

Environmental fate

Bioconcentration factor (BCF)	<3 (no guideline followed) Klimisch score: 2	[1]
Ready biodegradability	Readily biodegradable (EU Method C.4-C Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) Klimisch score: 1	[1]
Adsorption/desorption	log K_{OC}: 6 (PCKOCWIN version 2.00) Klimisch score: 2	[2]

PBT

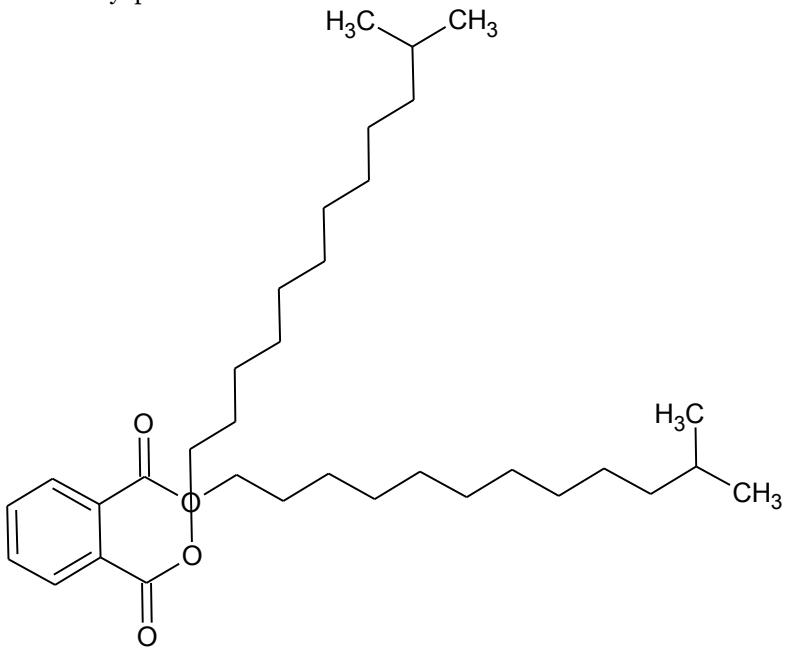
REACH registration dossier	not P/vP, not B/vB, not T
QSAR	P: Pos; B: Neg; T: ??; BCF: 230 Fish ChV (mg/L): ?? Half-life (Water, days): 38 Half-life (Soil, days): 75 Half-life (Sediment, days): 340 Half-life (Air, days): 0.67

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	53 metabolites formed. Of these: 47 bioavailable and 6 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	2 metabolites formed. Of these: 1 bioavailable and 1 not-bioavailable. Monoesters formed.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	6 metabolites formed. Of these: 4 bioavailable and 2 not-bioavailable. Monoesters formed.
Skin metabolism	17 metabolites formed. Of these: 11 bioavailable and 6 not-bioavailable. Monoesters formed.

Diisotridecyl phthalate (DITP)

Identification of substance

CAS No.	27253-26-5
EINECS No.	248-368-3
IUPAC name	Diisotridecyl phthalate
Structure	
SMILES	CC(C)CCCCCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCCCCC(C)C

REACH

Registration	Full
Submission	Joint submission
Total tonnage	1,000-10,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (2)
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	Yes
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	Yes

Physico-chemical characteristics

Molecular weight	530.84 g/mole	
Vapour pressure	<0.001 Pa, 38°C (ASTM D 2819) Klimisch score: 2	[1]
Henry's law constant	275 Pa m³/mol, 25°C (estimated by calculation) Klimisch score: 2	[2]
Water solubility	Insoluble (<0.1 mg/L) (ASTM E 1148) Klimisch score: 2	[1]
Log K_{OW}	13.5, 23°C, pH 7 (ASTM-E1147 Standard Test Method for Partition Coefficient (N-Octanol/Water) Estimation by Liquid Chromatography) Klimisch score: 2	[1]

Ecotoxicological data

Algae	EC50 (*Selenastrum capricornutum*, 8 days): >0.6 mg/L* (USEPA 600/9-78-018, Printz Algal Assay Bottle Test. 1978) (Read-across) Klimisch score: 1	[7]
Crustaceans	LC50 (*Daphnia magna*, 48 hours): >0.05 mg/L (USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975) (Read-across) Klimisch score: 1	[7]
	NOEC (*Daphnia magna*, 21 days): 0.052 mg/L (US EPA Environmental Effects Test Guidelines, ES-1, EPA 560/6-82-002) (Read-across) Klimisch score: 1	[7]
Fish	LC50 (*Oncorhynchus mykiss*, 96 hours): >0.15 mg/L* (USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians) (Read across) Klimisch score: 1	[7]
	NOEC (*Oncorhynchus mykiss*, 120 days): 0.3 mg/L* (US Environmental Protection Agency, Toxic Substance Control Act (EPA-TSCA) 40 CFR, Part 797.1600) (Read across) Klimisch score: 1	[7]
Terrestrial plants	EC50 (*Lolium species*, 5 days): >8551 mg/kg artificial soil (d.w.) (U.S. EPA-600/3-88/029 Protocols for Short Term Toxicity Screening of Hazardous Waste Sites (NTIS / PB88-235510/AS)) (Read-across) Klimisch score: 1	[7]
Soil macroorganisms	LC50 (*Eisenia fetida*, 14 days): >8435 mg/kg soil dw (OECD Guideline 207 Earthworm, Acute Toxicity Tests) (Read-across) Klimisch score: 1	[7]
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	-	

Environmental fate

Bioconcentration factor (BCF)	1 L/kg (no guideline followed) (Read-across) Klimisch score: 2	[7]
Ready biodegradability	Inherently biodegradable, not fulfilling specific criteria (OECD Guideline 301 F) (Read-across) Klimisch score: 1	[7]
Adsorption/desorption	log K_{OC}: 6.08 (EPA OTS 796.2750) (Read across) Klimisch score: 2	[7]

PBT

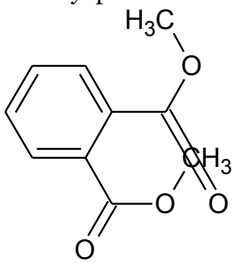
REACH registration dossier	-
QSAR	P: Pos; B: Neg; T: ??; BCF: 11 Fish ChV (mg/L): ?? Half-life (Water, days): 38 Half-life (Soil, days): 75 Half-life (Sediment, days): 340 Half-life (Air, days): 0.46

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	69 metabolites formed. Of these: 57 bioavailable and 12 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	6 metabolites formed. Of these: 1 bioavailable and 5 not-bioavailable. Monoesters formed.
Skin metabolism	24 metabolites formed. Of these: 8 bioavailable and 16 not-bioavailable. Monoesters formed.

Dimethyl phthalate (DMP)

Identification of substance

CAS No.	131-11-3
EINECS No.	205-011-6
IUPAC name	Dimethyl phthalate
Structure	
SMILES	O=C(OC)c(c(ccc1)C(=O)OC)c1

REACH

Registration	Full
Submission	Joint submission
Total tonnage	10,000-100,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (1122). 1 out of appro.x 1200 claim Repr 2 H361
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	Yes
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	194.19 g/mole	
Vapour pressure	0.0013 hPa, 20°C (OECD Guideline 104) Klimisch score: 2	[1]
Henry's law constant	0.023 Pa m³/mol, 25°C (HENRY v3.10 (Bond estimation method)) Klimisch score: 2	[4]
Water solubility	4,000 mg/L, 25°C (measured) Klimisch score: 2	[1]
Log K_{OW}	1.54, 25°C (OECD Guideline 107) Klimisch score: 2	[1]

Ecotoxicological data

Algae	EC50 (*Scenedesmus subspicatus*, 72 hours): 204 mg/L (German national standard DIN 38412 L9) Klimisch score: 2	[1]
Crustaceans	LC50 (*Daphnia magna*, 48 hours): > 52 mg/L (EG&G Bionomics Protocol for Static Acute Toxicity Tests with the Water Flea (*Daphnia magna*)) Klimisch score: 1	[1]
	NOEC (*Daphnia magna*, 21 days): 9.6 mg/L (Full life-cycle study, comparable to EPA guideline OTS 797.1330) Klimisch score: 2	[1]
Fish	LC50 (*pimephales promelas*, 96 hour): 39 mg/L (EG&G, Bionomics Methods for Conducting Flow-Through Toxicity Tests with Freshwater Fish) Klimisch score: 1	[1]
	NOEC (*Oncorhynchus mykiss*, 102 days): 11 mg/L (EPA-TSCA 40 CFR, Part 797.1600) Klimisch score: 2	[1]
Terrestrial plants	-	
Soil macroorganisms	LC50 (*Eisenia fetida*, 14 days): 3160 mg/kg soil dw (ECC artificial soil) Klimisch score: 2	[1]
PNEC (fresh water)	0.192 mg/L (Assessment factor: 50)	
PNEC (marine water	0.0192 mg/L (Assessment factor: 500)	
PNEC (fresh water sediment)	1.403 mg/kg sediment dw	
PNEC (marine water sediment)	-	
PNEC (soil)	3.16 mg/kg soil dw	

Environmental fate

Bioconcentration factor (BCF)	57 (Flow-through bioaccumulation fish-test comparable to OECD guideline 305) Klimisch score: 2	[1]
Ready biodegradability	Readily biodegradable (OECD Guideline 301 E) Klimisch score: 2	[1]
Adsorption/desorption	K_{OC}: 37.09 (PCKOCWIN v1.66) Klimisch score: 2	[2]

PBT

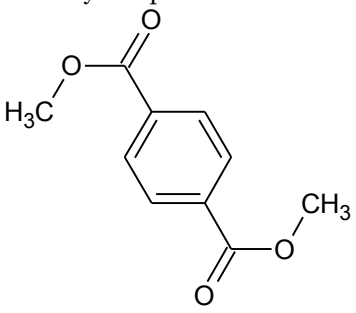
REACH registration dossier	Not vPvB; not T
QSAR	P: Neg; B: Neg; T: Pos; BCF: 5.3 Fish ChV (mg/L): 3.3 Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 28

QSAR bioavailability

Lipinski	Bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	5 metabolites formed. Of these: 5 bioavailable and 0 not-bioavailable. Monoesters formed.
Microbial metabolism (simulated)	15 metabolites formed. Of these: 15 bioavailable and 0 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	3 metabolites formed. Of these: 3 bioavailable and 0 not-bioavailable. Monoesters formed.
Skin metabolism	2 metabolites formed. Of these: 2 bioavailable and 0 not-bioavailable. Monoesters formed.

Dimethyl terephthalate (DMTP)

Identification of substance

CAS No.	120-61-6
EINECS No.	204-411-8
IUPAC name	Dimethyl terephthalate
Structure	
SMILES	O=C(OC)c(ccc(c1)C(=O)OC)c1

REACH

Registration	Full
Submission	Joint submission
Total tonnage	100,000-1,000,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (316); No classification for reproduction toxicity
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	194.19 g/mole	
Vapour pressure	0.000139 kPa, 293.15 K (EU Method A.4 (Vapour Pressure)) Klimisch score: 2	[1]
Henry's law constant	0.870696 Pa m³/mol, 20°C (Calculated using experimental values for solubility and vapour pressure using a recognised method) Klimisch score: 2	[4]
Water solubility	31 mg/L, 20°C, pH 5.4 (OECD Guideline 105) Klimisch score: 2	[1]
Log K_{OW}	2.21, 23°C (OECD Guideline 107) Klimisch score: 2	[1]

Ecotoxicological data

Algae	EC50 (*Desmodesmus subspicatus*, 72 hours): >29 mg/L (OECD Guideline 201) Klimisch score: 1	[1]
Crustaceans	EC50 (*Daphnia magna*, 48hours): >23.5 mg/L (OECD Guideline 202) Klimisch score: 1	[1]
	NOEC (*Daphnia magna*, 21 days): 1.72 mg/L (OECD Guideline 211) Klimisch score: 1	[1]
Fish	LC50 (*Danio rerio*, 96 hours): 13 mg/L (OECD Guideline 203) Klimisch score: 2	[1]
	-	
Terrestrial plants	-	
Soil macroorganisms	-	
PNEC (fresh water)	0.0172 mg/L (Assessment factor: 100)	
PNEC (marine water	0.00172 mg/L (Assessment factor: 1000)	
PNEC (fresh water sediment)	0.25 mg/kg sediment dw	
PNEC (marine water sediment)	0.025 mg/kg sediment dw	
PNEC (soil)	0.04 mg/kg soil dw (Assessment factor: -)	

Environmental fate

Bioconcentration factor (BCF)	-	
Ready biodegradability	Readily biodegradable (ISO Draft (BOD Test for Insoluble Substances)) Klimisch score: 1	[1]
Adsorption/desorption	K_{OC}: 30.96 (Sabljic molecular connectivity index)/109.3 (Calculated from measured log K_{OW} for dimethylterephthalate held in the KOWWIN database) (EPI-SUITE) (QSAR) Klimisch score: 2	[8]

PBT

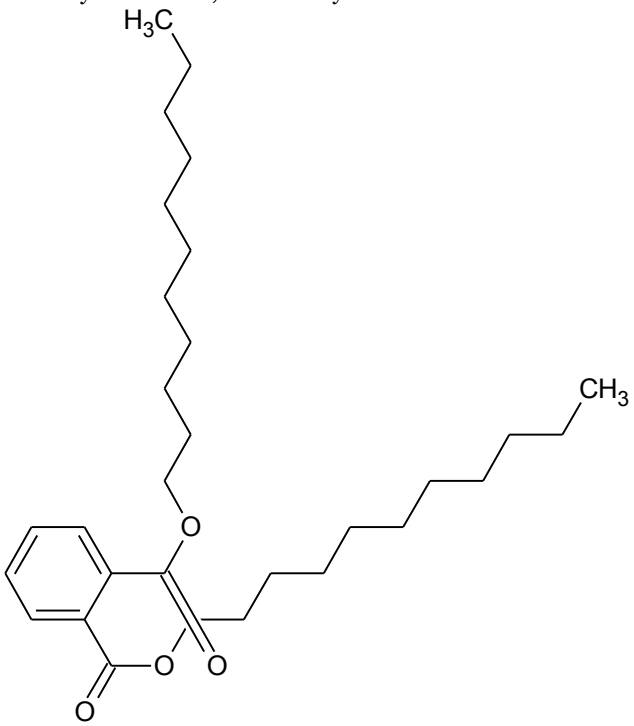
REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Neg; B: Neg; T: Pos; BCF: 14 Fish ChV (mg/L): 3.3 Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 28

QSAR bioavailability

Lipinski	Bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	23 metabolites formed. Of these: 23 bioavailable and 0 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	3 metabolites formed. Of these: 3 bioavailable and 0 not-bioavailable. Monoesters formed.
Skin metabolism	2 metabolites formed. Of these: 2 bioavailable and 0 not-bioavailable. Monoesters formed.

Diundecyl phthalate (DUP)

Identification of substance

CAS No.	3648-20-2
EINECS No.	222-884-9
IUPAC name	Diundecyl benzene-1,2-dicarboxylate
Structure	
SMILES	O=C(OCCCCCCCCCCC)c(c(ccc1)C(=O)OCCCCCCCCCCC)c1

REACH

Registration	Full
Submission	Joint submission
Total tonnage	1,000-10,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (53); Aquatic chronic 1 H410 (1)
Wide dispersive end use opened/closed	No
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	474.73 g/mole	
Vapour pressure	<7 hPa, 25°C (EC/440/2008) Klimisch score: 1	[1]
Henry's law constant	5.68 Pa m³/mol, 25°C (ENRYWIN Program (v 3.20)) Klimisch score: 2	[2]
Water solubility	1.11 mg/L, 25°C (Company SOP approved by CMA used) Klimisch score: 2	[1]
Log K_{OW}	8.7, 55°C, pH 7.7 (OECD Guideline 117) Klimisch score: 1	[1]

Ecotoxicological data

Algae	EC50 (*Pseudokirchnerella subcapitata*, 72 hours): >3.3 mg/L* (OECD Guideline 201) Klimisch score: 1	[1]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): >0.022 mg/L (EPA OTS 797.1300 (Aquatic Invertebrate Acute Toxicity Test, Freshwater Daphnids)) Klimisch score: 2	[1]
	NOEC (*Daphnia magna*, 21 days): 0.059 mg/L (no guideline followed) Klimisch score: 2	[1]
Fish	LC50 (*Oncorhynchus mykiss*, 96 hours): 1.4 mg/L* (EPA-660/3-75-009) Klimisch score: 2	[1]
	NOEC (*Oncorhynchus mykiss*, 155 days): 0.3 mg/L (EPA OPPTS 850.1400) Klimisch score: 1	[1]
Terrestrial plants	LC50 (*Triticum aestivum*, 19 days): >100 mg/kg soil dw (OECD guideline 208) (Read across) Klimisch score: 2	[7]
Soil macroorganisms	LC10 (*earthworm*, 14 days): >1000 mg/kg soil dw (EU Method C.8 (Toxicity for Earthworms: Artificial Soil Test)) (Read across) Klimisch score: 2	[7]
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	-	

Environmental fate

Bioconcentration factor (BCF)	21.4 L/kg wet weight (EPIWIN (v 4.0), WSKOW (v1.41)) Klimisch score: 2	[2]
Ready biodegradability	Readily biodegradable, but failing 10-day window (EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test)) Klimisch score: 1	[1]
Adsorption/desorption	log $K_{OC,soil}$: 21.41 (EU Method C.19 (Estimation of the Adsorption Coefficient (K_{OC}) on Soil and Sewage Sludge Using High Performance Liquid Chromatography (HPLC))) Klimisch score: 1	[1]

PBT

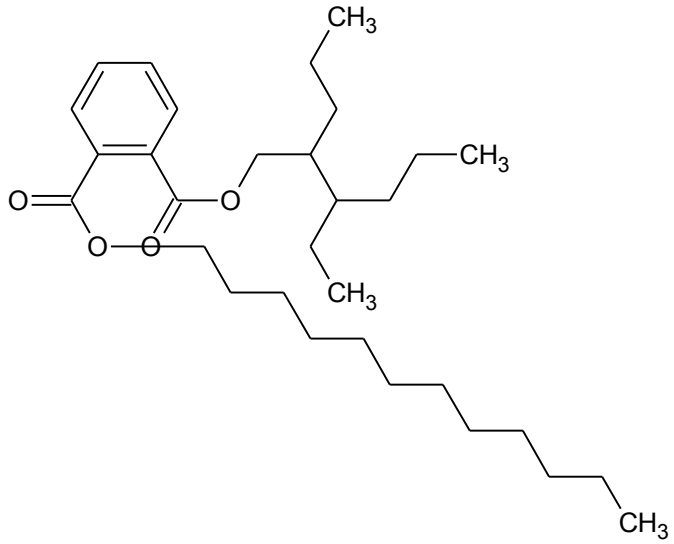
REACH registration dossier	-
QSAR	P: Neg; B: Neg; T: ???; BCF: 21 Fish ChV (mg/L): ?? Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 0.54

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	64 metabolites formed. Of these: 40 bioavailable and 24 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	5 metabolites formed. Of these: 4 bioavailable and 1 not-bioavailable. Monoesters formed.
Skin metabolism	8 metabolites formed. Of these: 5 bioavailable and 3 not-bioavailable. Monoesters formed.

Diundecyl phthalate, branched and linear (DIUP)

Identification of substance

CAS No.	85507-79-5
EINECS No.	287-401-6
IUPAC name	1,2-benzenedicarboxylic acid, di-C10-12-branched alkyl esters, C11-rich
Structure	
SMILES	O=C(c1ccccc1C(=O)OCCCCCCCCCCCC)OCC(C(CC)CCC)CCC

REACH

Registration	Full
Submission	Joint submission
Total tonnage	1,000-10,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (19)
Wide dispersive end use opened/closed	No
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	488.76 g/mole	
Vapour pressure	0.00000000497 hPa, 25°C (QSPR (quantitative structure-property relationship)) Klimisch score: 2	[9]
Henry's law constant	50.5 Pa m³/mol, 25°C (QSPR (quantitative structure-property relationship)) Klimisch score: 2	[2]
Water solubility	0.00441 µg/L, 25°C, pH 7 (QSPR (quantitative structure-property relationship)) Klimisch score: 2	[9]
Log Kow	10.33, 25°C, pH 7 (QSPR (quantitative structure-property relationship)) Klimisch score: 2	[9]

Ecotoxicological data

Algae	EC50 (*Selenastrum capricornutum*, 8 days): >2.1 mg/L* (USEPA 600/9-78-018, Printz Algal Assay Bottle Test. 1978) (Read-across) Klimisch score: 1	[7]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): >0.9 mg/L* (OECD Guideline 202) Klimisch score: 1	[1]
	NOEC (*Daphnia magna*, 21 days): 0.9 mg/L* (OECD Guideline 211) Klimisch score: 1	[1]
Fish	LC50 (*Oncorhynchus mykiss*, 96 hours): >1.4 mg/L* (USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians) (Read-across) Klimisch score: 1	[7]
	NOEC (*Oryzias latipes*, 284 days): >= 19.2 <= 22.7 other: ug/g feed (OECD Guideline 210) (Read-across) Klimisch score: 2	[7]
Terrestrial plants	EC50 (*Lactuca sativa*, 5 days): >8551 other: mg/kg artificial soil (d.w.) (U.S. EPA-600/3-88/029 Protocols for Short Term Toxicity Screening of Hazardous Waste Sites (NTIS / PB88-235510/AS)) (Read-across) Klimisch score: 1	[7]
Soil macroorganisms	LC50 (*Eisenia fetida*, 14 days): >7664 other: mg/kg natural soil dw (OECD Guideline 207) (Read-across) Klimisch score: 1	[7]
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	-	

Environmental fate

Bioconcentration factor (BCF)	3.2 (BCFWIN subroutine (version 2.15)) Klimisch score: 2	[2]
Ready biodegradability	Inherently biodegradable (OECD Guideline 301 F) Klimisch score: 2	[1]
Adsorption/desorption	log K_{OC}: > 5.46 < 6.08 (EPA OTS 796.2750 (Sediment and Soil Adsorption Isotherm)) (Read-across) Klimisch score: 2	[7]

PBT

REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Pos; B: Neg; T: ??; BCF: 14 Fish ChV (mg/L): ?? Half-life (Water, days): 38 Half-life (Soil, days): 75 Half-life (Sediment, days): 340 Half-life (Air, days): 0.5

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	585 metabolites formed. Of these: 376 bioavailable and 209 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	40 metabolites formed. Of these: 25 bioavailable and 15 not-bioavailable. Monoesters formed.
Skin metabolism	92 metabolites formed. Of these: 57 bioavailable and 35 not-bioavailable. Monoesters formed.

Ester reaction products of 1,4-benzenedicarboxylic acid with C11-14 iso-alcohols, C13-rich

Identification of substance

CAS No.	xx
EINECS No.	416-740-6
IUPAC name	Ester reaction products of 1,4-benzenedicarboxylic acid with C11-14 iso-alcohols, C13-rich
Structure	N/A
SMILES	O=C(OCCCCCCCCCCCCC)c(c(ccc1)C(=O)OCCCCCCCCCCCCC)c1

REACH

Registration	Full
Submission	Joint submission
Total tonnage	100-1,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (4)
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	Yes
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	530.84 g/mole	
Vapour pressure	0.00042 Pa, 25°C (EU Method A.4 (Vapour Pressure)) Klimisch score: 1	[1]
Henry's law constant	0.0424 atm m³/mol, 25 °C (EPI Suite V3.12) Klimisch score: 2	[2]
Water solubility	> 0.000026 < 0.00068 mg/L, 25°C (calculated using method of Yalkowsky and McKay) Klimisch score: 2	[1]
Log K_{OW}	>= 9.5 <= 11, , 25°C (EU Method A.8 (Partition Coefficient) HPLC method) Klimisch score: 1	[1]

Ecotoxicological data

Algae	EL50 (*Selenastrum sp.*, 72 hours): >5008 mg/L* (OECD Guideline 201) Klimisch score: 2	[1]
Crustaceans	EL50 (*Daphnia magna*, 48 hours): >5100 mg/L* (OECD Guideline 202) Klimisch score: 1	[1]
	NOEL (*Daphnia magna*, 21 days): >1 µg/L* (OECD Guideline 211) Klimisch score: 1	[7]
Fish	LL50 (*Oncorhynchus mykiss*, 96 hours): >5008 mg/L* (OECD Guideline 203) Klimisch score: 1	[1]
	NOEL (, 71 days): >0.35 mg/L* (EPA Bioassay for egg and fry stages of freshwater fish) Klimisch score: 1	[7]
Terrestrial plants	EL50 (*Glycine max*, 14 days): >1500 µg/L (EPA Early seedling growth toxicity test EG-13 (1986)) Klimisch score: 1	[7]
Soil macroorganisms	LL50 (*Eisenia fetida*, 14 days): >10000 mg/kg natural and artificial soil d.w. (OECD Guideline 207) Klimisch score: 1	[10]
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	-	

Environmental fate

Bioconcentration factor (BCF)	0.8953 (EPiSuite 4.0 BCFBAF v3.00) Klimisch score: 2	[2]
Ready biodegradability	Inherently biodegradable (OECD Guideline 301 B) Klimisch score: 1	[1]
Adsorption/desorption	log K_{OC}: 8.15 (EPI Suite v4.0) Klimisch score: 2	[2]

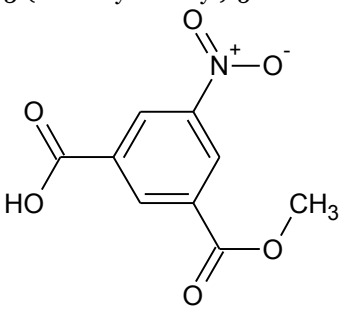
PBT

REACH registration dossier	
QSAR	P: Neg; B: Neg; T: ??; BCF: 9.2 Fish ChV (mg/L): ?? Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 0.46

QSAR bioavailability	
Lipinski	n.d.
Mammalian metabolism	n.d.
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	n.d.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	n.d.
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	n.d.
Skin metabolism	n.d.

Methyl 5-nitrohydrogen.isophthalate

Identification of substance

CAS No.	1955-46-0
EINECS No.	217-793-6
IUPAC name	3-(methoxycarbonyl)-5-nitrobenzoic acid
Structure	
SMILES	O=C(OC)c(cc(N(=O)=O)cc1C(=O)O)c1

REACH

Registration	Full
Submission	Joint submission
Total tonnage	1-10 tonnes per annum
Harmonised classification	
Notified classification	Skin Irrit. 2 H315 Eye Irrit. 2 H319 STOT SE 3 H335 (15); Not classified (3). No classification of reproduction toxicity
Wide dispersive end use opened/closed	No
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	225.16 g/mole	
Vapour pressure	0.0000000856 mm Hg, 25°C ((ACD/Labs) Software V11.02) Klimisch score: 2	[2]
Henry's law constant	1.28E-012 atm-m³/mole, 25°C (Estimation Programs Interface Suite™ United States Environmental Protection Agency, Washington, DC, USA. version 4.1) Klimisch score: 2	[2]
Water solubility	1,900 mg/L, 25 °C (-) Klimisch score: 1	[1]
Log Kow	1.65, 25°C (-) Klimisch score: 1	[1]

Ecotoxicological data

Algae	EC50 (-, 72 hours): 24.85464 mg/L (QSAR Toolbox 2.3.0.1132 prediction for EC50 read across evaluation for 1955-46-0) (Read-across) Klimisch score: 2	[10]
Crustaceans	EC50 (*Daphnia magna*, 24 hours): 26.5849 mg/L (QSAR Toolbox 2.3.0.1132 prediction for EC50 read across evaluation for 1955-46-0) (Read-across) Klimisch score: 2	[10]
	ChV (*Daphnia magna*, 21 days): 887.873 mg/L (ECOSAR Version 1.10) Klimisch score: 2	[2]
Fish	EC50 (-, 48 hours): 30.42095 mg/L (QSAR Toolbox 2.3.0.1132 prediction for EC50 read across evaluation for 1955-46-0) (Read-across) Klimisch score: 2	[10]
	LC50 (fish, 14 days): 167000 mg/L* (ECOSAR Version 1.10) Klimisch score: 2	[2]
Terrestrial plants	IC50 (*Zea mays*, 8 days): 27.44769 mg/L (QSAR Toolbox 2.3.0.1132 prediction for IC50 read across evaluation for 1955-46-0) (Read-across) Klimisch score: 2	[10]
Soil macroorganisms	LC50 (earthworm, 14 days): 41695.367 mg/L (ECOSAR Version 1.10) Klimisch score: 2	[2]
PNEC (fresh water)	57.0338 mg/L (Assessment factor: 10)	
PNEC (marine water	5.70338 mg/L (Assessment factor: 100)	
PNEC (fresh water sediment)	56.41498327 mg/kg sediment dw	
PNEC (marine water sediment)	56.41498327 mg/kg sediment dw	
PNEC (soil)	41.695367 mg/kg soil dw (Assessment factor: 1000)	

Environmental fate

Bioconcentration factor (BCF)	2.44, 25°C, pH 4 ((ACD/Labs) Software V11.02) Klimisch score: 2	[2]
Ready biodegradability	Readily biodegradable (BIOWIN (v4.10)) Klimisch score: 2	[2]
Adsorption/desorption	K_{OC}: 11.846, 25°C (Estimation Programs Interface Suite™ United States Environmental Protection Agency, Washington, DC, USA. version 4.1) Klimisch score: 2	[2]

PBT

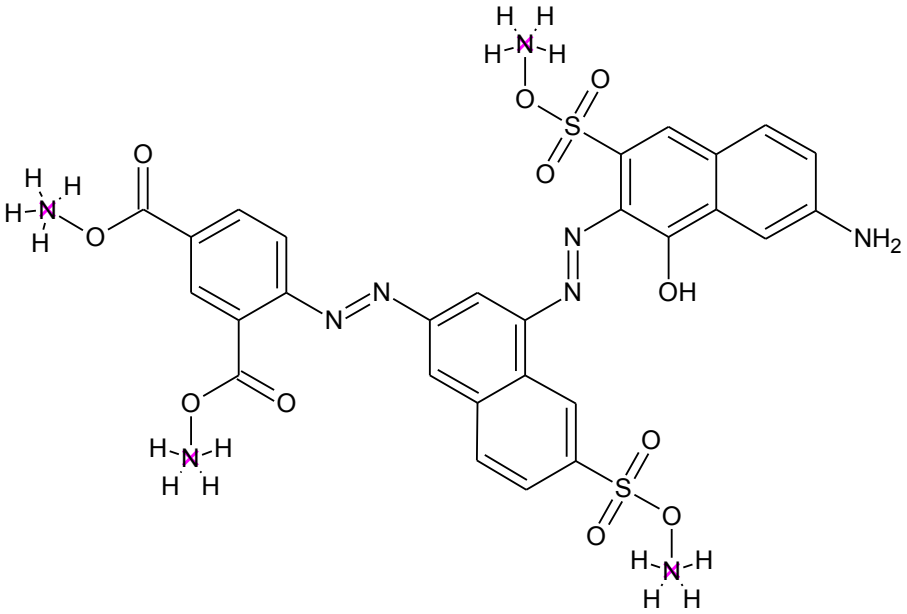
REACH registration dossier	-
QSAR	P: Neg; B: Neg; T: Neg; BCF: 3.2 Fish ChV (mg/L): 46 Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 21

QSAR bioavailability

Lipinski	Bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	50 metabolites formed. Of these: 49 bioavailable and 1 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	4 metabolites formed. Of these: 4 bioavailable and 0 not-bioavailable. Monoesters formed.
Skin metabolism	2 metabolites formed. Of these: 2 bioavailable and 0 not-bioavailable. Monoesters formed.

Tetraammonium 5-(4-(7-amino-1-hydroxy-3-sulfonato-2-naphthylazo)-6-sulfonato-1-naphthylazo)isophthalate

Identification of substance

CAS No.	128351-36-0
EINECS No.	405-130-5
IUPAC name	-
Structure	
SMILES	c1cc(C(=O)ON(H)(H)(H)(H))cc(C(=O)ON(H)(H)(H)(H))c1N=Nc2cc3ccc(S(=O)(=O)ON(H)(H)(H)(H))cc3c(N=Nc4c(O)c5cc(N)ccc5cc4(S(=O)(=O)ON(H)(H)(H)(H)))c2

REACH

Registration	NONS
Submission	Individual submission
Total tonnage	Tonnage sata confidential
Harmonised classification	Skin sens 1; H317
Notified classification	
Wide dispersive end use opened/closed	
Wide dispersive end use closed	
Wide dispersive service life opened/closed	
Wide dispersive service life closed	

Physico-chemical characteristics

Molecular weight	-	
Vapour pressure	-	
	Klimisch score: -	
Henry's law constant	-	
Water solubility	-	
	Klimisch score: -	
Log K_{OW}	-	
	Klimisch score: -	

Ecotoxicological data

Algae	EC50 (Green algae, 96 hours): 0.04 mg/L* (-) Klimisch score: 4	[17]
Crustaceans	LC50 (Daphnid, 48 hours): 0.362 mg/L* (-) Klimisch score: 4	[13]
	ChV (Daphnid, 21 days): 0.0008 mg/L (-) Klimisch score: 4	[17]
Fish	LC50 (fish, 96 hours): 0.073 mg/L* (ECOSAR) Klimisch score: 4	[17]
	ChV (2-33 days; fish): 0.0002 mg/L* (ECOSAR) Klimisch score: 4	[17]
Terrestrial plants	-	
Soil macroorganisms	-	
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	- (Assessment factor: -)	

Environmental fate

Bioconcentration factor (BCF)	-
Ready biodegradability	-
Adsorption/desorption	-

PBT

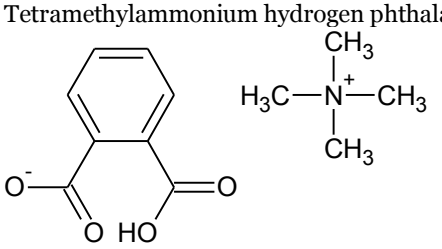
REACH registration dossier	-
QSAR	P: -; B: -; T: -; BCF: - Fish ChV (mg/L): - Half-life (Water, days): - Half-life (Soil, days): - Half-life (Sediment, days): - Half-life (Air, days): -

QSAR bioavailability

Lipinski	n.d.
Mammalian metabolism	
Microbial metabolism (observed)	
Microbial metabolism (simulated)	
Rat In vivo metabolism (observed)	
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	
Rat Liver S9 metabolism (simulated)	
Skin metabolism	

Tetramethylammonium hydrogen phthalate

Identification of substance

CAS No.	79723-02-7
EINECS No.	416-900-5
IUPAC name	Tetramethylammonium hydrogen phthalate
Structure	
SMILES	C[N+](C)(C)C.OC(=O)C1=CC=CC=C1C([O-])=O

REACH

Registration	NONS
Submission	Individual submission
Total tonnage	Tonnage data confidential
Harmonised classification	Acute tox 3; H301 STOT RE 2; H373 Aquatic Acute 1; H400
Notified classification	-
Wide dispersive end use opened/closed	No
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	239.27 g/mole	
Vapour pressure	<= 0.00001 Pa, 25°C (EU Method A.4 (Vapour Pressure)) Klimisch score: 2	[1]
Henry's law constant	-	
Water solubility	725 g/L, 20°C, pH 5.4 Klimisch score: 2	[1]
Log K_{OW}	-1.24, 23°C (EU Method A.8 (Partition Coefficient)) Klimisch score: 2	[1]

Ecotoxicological data

Algae	EC50 (*Scenedesmus subspicatus*, 72 hours): 0.32 mg/L (OECD Guideline 201) Klimisch score: 2	[1]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): 3.3 mg/L (OECD Guideline 202) Klimisch score: 2	[1]
	-	
Fish	-	
	-	
Terrestrial plants	-	
Soil macroorganisms	-	
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	-	

Environmental fate

Bioconcentration factor (BCF)	-	
Ready biodegradability	Readily biodegradable (OECD Guideline 301 D) Klimisch score: 2	[1]
Adsorption/desorption	-	

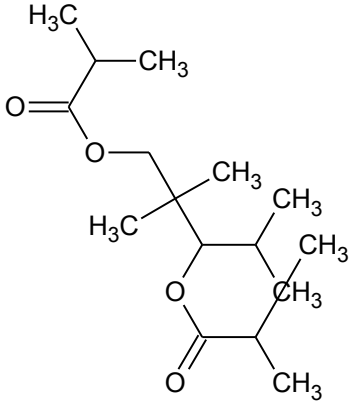
PBT

REACH registration dossier	-
QSAR	P: Neg; B: Neg; T: Neg; BCF: 3.2 Fish ChV (mg/L): 250000 Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 16

QSAR bioavailability	
Lipinski	n.d.
Mammalian metabolism	
Microbial metabolism (observed)	
Microbial metabolism (simulated)	
Rat In vivo metabolism (observed)	
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	
Rat Liver S9 metabolism (simulated)	
Skin metabolism	

1-isopropyl-2,2-dimethyltrimethylene diisobutyrate (TXIB)

Identification of substance

CAS No.	6846-50-0
EINECS No.	229-934-9
IUPAC name	2,2,4-trimethylpentane-1,3-diyl bis(2-methylpropanoate)
Structure	
SMILES	O=C(OCC(C)(C)C(OC(=O)C(C)C)C(C)C)C(C)C

REACH

Registration	Full
Submission	Joint submission
Total tonnage	1,000-10,000 tonnes per annum
Harmonised classification	
Notified classification	
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	Yes
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	286.42 g/mole	
Vapour pressure	<1.5 Pa, 25°C (EU Method A.4) Klimisch score: 2	[1]
Henry's law constant	-	
Water solubility	12.7 mg/L, 27.5°C, pH 3.6 - 4.6 (no guideline followed) Klimisch score: 2	[1]
Log K_{OW}	4.49, 25°C, pH 7 (QSAR (SPARC) used, and acceptable in accordance with REACH Annex XI) (WOE)	[6]

	Klimisch score: 2	

Ecotoxicological data

Algae	EC50 (*Selenastrum capricornutum*, 72 hours): >7.49 mg/L (OECD Guideline 201) Klimisch score: 1	[1]
Crustaceans	EC50 (*Asellus intermedius*, 96 hours): >1.55 mg/L (ASTM Standard E 729-80. 1985) (WOE) Klimisch score: 2	[12]
	NOEC (*Daphnia magna*, 21 days): 0.7 mg/L (the study is equivalent to the current OECD Guideline 211, *Daphnia magna* Reproduction Test) Klimisch score: 1	[1]
Fish	NOEC (*Lepomis macrochirus*, 96 hours): >=6 mg/L (OECD Guideline 203) Klimisch score: 1	[1]
	-	
Terrestrial plants	-	
Soil macroorganisms	-	
PNEC (fresh water)	0.014 mg/L (Assessment factor: 50)	
PNEC (marine water	0.0014 mg/L (Assessment factor: 500)	
PNEC (fresh water sediment)	1.15 mg/kg sediment dw	
PNEC (marine water sediment)	-	
PNEC (soil)	0.926 mg/kg soil dw (Assessment factor: -)	

Environmental fate

Bioconcentration factor (BCF)	1.95 - 5340 (OECD Guideline 305) Klimisch score: 1	[1]
Ready biodegradability	Readily biodegradable but failing 10-day window (OECD Guideline 301 B) Klimisch score: 1	[1]
Adsorption/desorption	log K_{OC}: 3.6 (QSAR (ACDLabs)) (WOE) Klimisch score: 2	[6]

PBT

REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Pos; B: Neg; T: Pos; BCF: 810 Fish ChV (mg/L): 0.031 Half-life (Water, days): 38 Half-life (Soil, days): 75 Half-life (Sediment, days): 340 Half-life (Air, days): 1.4

QSAR bioavailability

Lipinski	Bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	35 metabolites formed. Of these: 35 bioavailable and 0 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	7 metabolites formed. Of these: 7 bioavailable and 0 not-bioavailable. Monoesters formed.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	8 metabolites formed. Of these: 8 bioavailable and 0 not-bioavailable. Monoesters formed.
Skin metabolism	1 metabolites formed. Of these: 1 bioavailable and 0 not-bioavailable. Monoesters formed.

COMGHA

Identification of substance

CAS No.	736150-63-3
EINECS No.	451-530-8
IUPAC name	-
Structure	N/A
SMILES	-

REACH

Registration	Full
Submission	Individual submission
Total tonnage	1,000-10,000 tonnes per annum
Harmonised classification	
Notified classification	
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	- g/mole	
Vapour pressure	0.000000048 Pa, 20°C (OECD Guideline 104) Klimisch score: 1	[1]
Henry's law constant	-	
Water solubility	< 0.33 mg/L, 20°C, pH 6.8 (OECD Guideline 105) Klimisch score: 1	[1]
Log K_{OW}	6.4, 25°C (OECD Guideline 117) Klimisch score: 2	[1]

Ecotoxicological data

Algae	EC50 (*Selenastrum capricornutum*, 72 hours): 106 mg/L* (OECD Guideline 201) Klimisch score: 1	[1]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): 0.92 mg/L* (OECD Guideline 202) Klimisch score: 1	[1]
	NOEC (*Daphnia magna*, 21 days): >=70 µg/L (OECD Guideline 211) Klimisch score: 1	[1]
Fish	LC50 (*Danio rerio*, 96 hours): >0.28 mg/L (OECD Guideline 203) Klimisch score: 1	[1]
	NOEC (*Danio rerio*, 67 days): 32.1 µg/L (OECD Guideline 210) Klimisch score: 1	[1]
Terrestrial plants	EC50 (*Hordeum vulgare*, 22 days): 12.5 mg/kg soil dw (OECD Guideline 208) Klimisch score: 1	[1]
Soil macroorganisms	LC50 (*Eisenia fetida*, 14 days): >1000 mg/kg soil dw (OECD Guideline 207) Klimisch score: 1	[1]
PNEC (fresh water)	5 µg/L (Assessment factor: 10)	
PNEC (marine water	5 µg/L (Assessment factor: 100)	
PNEC (fresh water sediment)	28 mg/kg sediment dw	
PNEC (marine water sediment)	2.8 mg/kg sediment dw	
PNEC (soil)	0.02 mg/kg soil dw (Assessment factor: 100)	

Environmental fate

Bioconcentration factor (BCF)	981 (OECD Guideline 305) Klimisch score: 1	[1]
Ready biodegradability	Readily biodegradable (OECD Guideline 301 F) Klimisch score: 1	[1]
Adsorption/desorption	log K_{OC}: 5.4, 25°C (OECD Guideline 121) Klimisch score: 1	[1]

PBT

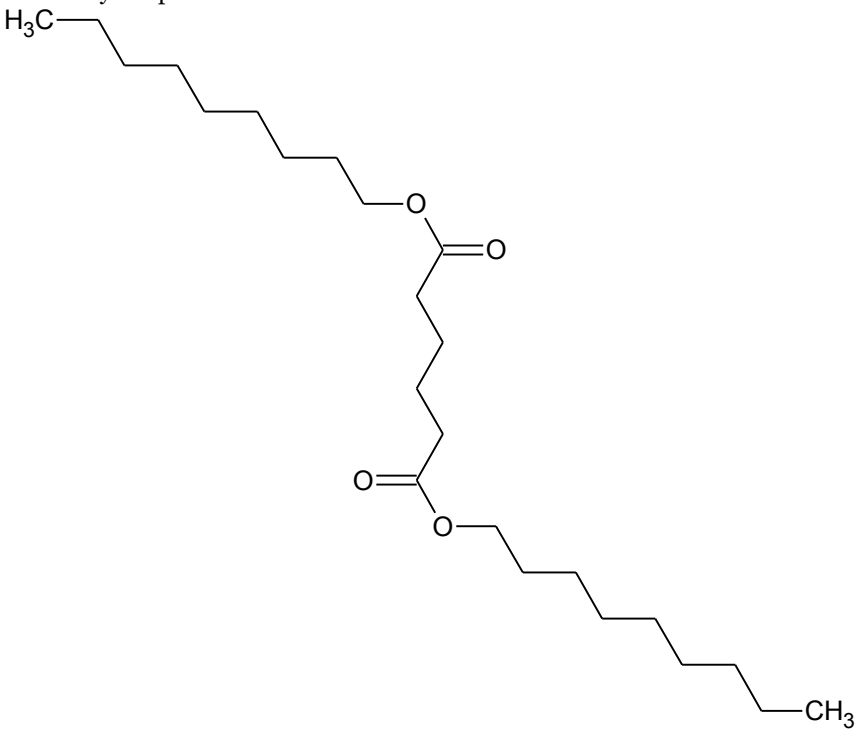
REACH registration dossier	-
QSAR	P: -; B: -; T: -; BCF: - Fish ChV (mg/L): - Half-life (Water, days): - Half-life (Soil, days): - Half-life (Sediment, days): - Half-life (Air, days): -

QSAR bioavailability

Lipinski	n.d.
Mammalian metabolism	
Microbial metabolism (observed)	
Microbial metabolism (simulated)	
Rat In vivo metabolism (observed)	
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	
Rat Liver S9 metabolism (simulated)	
Skin metabolism	

Diisononyl adipate (DINA)

Identification of substance

CAS No.	33703-08-1
EINECS No.	251-646-7
IUPAC name	Diisononyl adipate
Structure	
SMILES	O=C(OCCCCCCCCC)CCCCC(=O)OCCCCCCCCC

REACH

Registration	Full
Submission	Joint submission
Total tonnage	1,000 + tonnes per annum
Harmonised classification	
Notified classification	
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	Yes
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	398.63 g/mole	
Vapour pressure	0.000000002 hPa, 20°C (dynamic method) Klimisch score: 2	[1]
Henry's law constant	9.210442 Pa m³/mol, 25°C (SRC HENRYWIN v3.10) Klimisch score: 2	[2]
Water solubility	0.0032 mg/L, 22°C (Read-Across) Klimisch score: 2	[10]
Log K_{OW}	9.56 - 10.4, 25°C (OECD Guideline 117) Klimisch score: 2	[1]

Ecotoxicological data

Algae	EC50 (*Scenedesmus subspicatus*, 72 hours): >100 mg/L* (OECD Guideline 201) Klimisch score: 2	[1]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): >100 mg/L* (OECD Guideline 202) Klimisch score: 2	[1]
	NOEC (*Daphnia magna*, 21 days): >=0.77 mg/L* (OECD Guideline 211) (Read-across) Klimisch score: 2	[7]
Fish	LC50 (*Leuciscus idus*, 96 hours): >500 mg/L* (OECD Guideline 203) Klimisch score: 2	[1]
	-	
Terrestrial plants	-	
Soil macroorganisms	LC50 (*Eisenia fetida*, 14 days): 865 mg/kg soil dw (EU Method C.8) (Read-across) Klimisch score: 2	[7]
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	0.865 mg/kg soil dw (Assessment factor: -)	

Environmental fate

Bioconcentration factor (BCF)	27 (flow through system according to ASTM) (Read-across) Klimisch score: 2	[7]
Ready biodegradability	Readily biodegradable (OECD Guideline 301 F) Klimisch score: 2	[1]
Adsorption/desorption	log K_{OC}: 5.291 (SRC PCKOCWIN v1.66) Klimisch score: 2	[2]

PBT

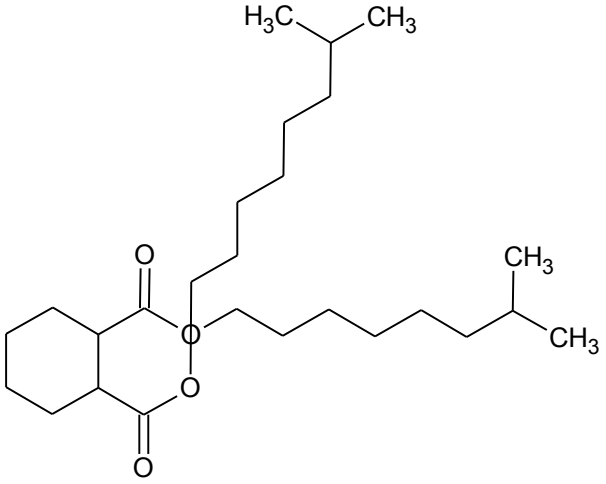
REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Neg; B: Neg; T: ??; BCF: 270 Fish ChV (mg/L): ?? Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 0.58

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	80 metabolites formed. Of these: 64 bioavailable and 16 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	15 metabolites formed. Of these: 13 bioavailable and 2 not-bioavailable. Monoesters formed.
Skin metabolism	27 metabolites formed. Of these: 19 bioavailable and 8 not-bioavailable. Monoesters formed.

DINCH

Identification of substance

CAS No.	166412-78-8
EINECS No.	431-890-2
IUPAC name	-
Structure	
SMILES	CC(C)CCCCCCOC(=O)C1CCCCC1C(=O)OCCCCCCC(C)C

REACH

Registration	NONS
Submission	Joint submission
Total tonnage	Tonnage data confidential
Harmonised classification	
Notified classification	
Wide dispersive end use opened/closed	No
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	424.67 g/mole	
Vapour pressure	0.00000022 hPa, 20°C (-) Klimisch score: -	[1]
Henry's law constant	7.15 Pa m³/mol, 25°C (EPIWIN) Klimisch score: -	[2]
Water solubility	<0.02 mg/L, 25°C, pH 6.3 - 7.4 (-) Klimisch score: -	[1]
Log K_{OW}	10, 25°C (-) Klimisch score: -	[1]

Ecotoxicological data

Algae	EC50 (*Scenedesmus subspicatus*, 72 hours): >100 mg/L* (-) Klimisch score: -	[1]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): >100 mg/L* (-) Klimisch score: -	[1]
	NOEC (*Daphnia magna*, 21 days): >=0.021 mg/L* (-) Klimisch score: -	[1]
Fish	LC50 (*Brachydanio rerio*, 96 hours): >100 mg/L* (-) Klimisch score: -	[1]
	-	
Terrestrial plants	EC50 (*Avena sativa; Brassica napus; Vicia sativa*, 20 days): > 1000 mg/kg soil dw (-) Klimisch score: -	[1]
Soil macroorganisms	LC50 (*Eisenia fetida*, 14 days): >1000 mg/kg (-) Klimisch score: -	[1]
PNEC (fresh water)	-	
PNEC (marine water	-	
PNEC (fresh water sediment)	-	
PNEC (marine water sediment)	-	
PNEC (soil)	10 mg/kg soil dw (Assessment factor: -)	

Environmental fate

Bioconcentration factor (BCF)	189.3 (-) Klimisch score: -	[1]
Ready biodegradability	Inherently biodegradable (no conclusion in dossier) (-) Klimisch score: -	[1]
Adsorption/desorption	log K_{OC}: 6.59 (-) Klimisch score: -	[1]

PBT

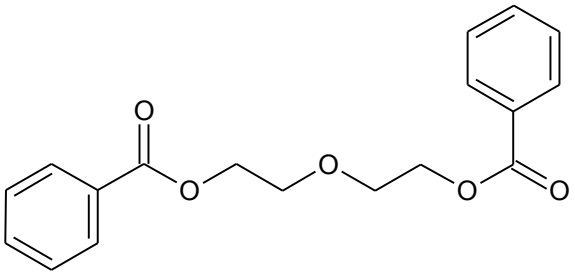
REACH registration dossier	-
QSAR	P: Pos; B: Neg; T: ??; BCF: 3.2 Fish ChV (mg/L): ?? Half-life (Water, days): 38 Half-life (Soil, days): 75 Half-life (Sediment, days): 340 Half-life (Air, days): 0.58

QSAR bioavailability

Lipinski	n.d.
Mammalian metabolism	
Microbial metabolism (observed)	
Microbial metabolism (simulated)	
Rat In vivo metabolism (observed)	
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	
Rat Liver S9 metabolism (simulated)	
Skin metabolism	

Oxydiethylene dibenzoate (DEGD)

Identification of substance

CAS No.	120-55-8
EINECS No.	204-407-6
IUPAC name	-
Structure	
SMILES	O=C(OCCOCCOC(=O)c(cccc1)c1)c(cccc2)c2

REACH

Registration	Full
Submission	Joint submission
Total tonnage	1,000-10,000 tonnes per annum
Harmonised classification	
Notified classification	
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	Yes
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	314.34 g/mole	
Vapour pressure	0.000018 Pa, 25°C (EU Method A.4) Klimisch score: 1	[1]
Henry's law constant	-	
Water solubility	38.3 mg/L, 20°C, pH 7 (OECD Guideline 105) Klimisch score: 1	[1]
Log K_{OW}	3.2, 20°C (OECD Guideline 117) Klimisch score: 1	[1]

Ecotoxicological data

Algae	EL50 (*Selenastrum capricornutum*, 72 hours): 10.94 mg/L (EU Method C.3) Klimisch score: 1	[1]
Crustaceans	EL50 (*Daphnia magna*, 48 hours): 6.7 mg/L (EU Method C.2) Klimisch score: 1 -	[1]
Fish	LL50 (*Oncorhynchus mykiss*, 96 hours): 2.9 mg/L (EU Method C.1) Klimisch score: 1 -	[1]
Terrestrial plants	-	
Soil macroorganisms	LC50 (*Eisenia fetida*, 14 days): >1,000 ppm (OECD Guideline 207) Klimisch score: 1	[1]
PNEC (fresh water)	2.9 µg/L (Assessment factor: 1,000)	
PNEC (marine water	0.29 µg/L (Assessment factor: 10,000)	
PNEC (fresh water sediment)	0.474 mg/kg sediment dw	
PNEC (marine water sediment)	0.0474 mg/kg sediment dw	
PNEC (soil)	1 mg/kg soil dw (Assessment factor: 1000)	

Environmental fate

Bioconcentration factor (BCF)	log BCF of 1.78 (EPISUITE v4.0 BCFBAF v3.00) (QSAR) Klimisch score: 2	[13]
Ready biodegradability	Readily biodegradable (EU Method C.4-C) Klimisch score: 1	[1]
Adsorption/desorption	log K_{OC}: 3.2, 20°C (OECD Guideline 121) Klimisch score: 1	[1]

PBT

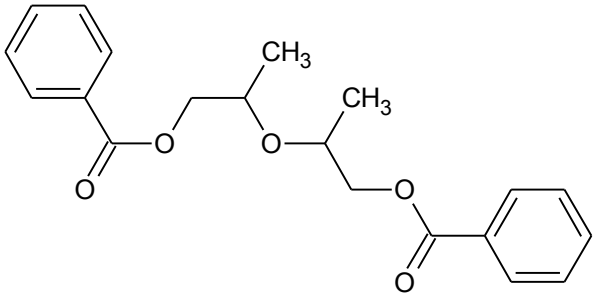
REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Neg; B: Neg; T: Pos; BCF: 47 Fish ChV (mg/L): 0.63 Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 0.83

QSAR bioavailability

Lipinski	Bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	32 metabolites formed. Of these: 32 bioavailable and 0 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	4 metabolites formed. Of these: 4 bioavailable and 0 not-bioavailable. Monoesters formed.
Skin metabolism	2 metabolites formed. Of these: 2 bioavailable and 0 not-bioavailable. Monoesters formed.

Oxydipropyl dibenzoate (DGD)

Identification of substance

CAS No.	27138-31-4
EINECS No.	248-258-5
IUPAC name	1-[2-(benzoyloxy)propoxy]propan-2-yl benzoate
Structure	
SMILES	O=C(c1ccccc1)OCC(OC(COC(=O)c2ccccc2)C)C

REACH

Registration	Full
Submission	Joint submission
Total tonnage	1,000-10,000 tonnes per annum
Harmonised classification	
Notified classification	
Wide dispersive end use opened/closed	No
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	342.39 g/mole	
Vapour pressure	0.00016 Pa, 25°C (EU Method A.4) Klimisch score: 1	[1]
Henry's law constant	-	
Water solubility	ca. 8.69 mg/L, 20°C, pH 7 (OECD Guideline 105) Klimisch score: 1	[1]
Log Kow	3.9, 20°C (OECD Guideline 117) (WOE) Klimisch score: 1	[12]

Ecotoxicological data

Algae	EL50 (*Selenastrum capricornutum*, 72 hours): 4.9 mg/L (EU Method C.3) Klimisch score: 1	[1]
Crustaceans	EL50 (*Daphnia magna*, 48 hours): 19.3 mg/L* (EU Method C.2) Klimisch score: 1 -	[1]
Fish	LC50 (*Pimephales promelas*, 96 hours): 3.7 mg/L (EU Method C.1) Klimisch score: 1 -	[1]
Terrestrial plants	-	
Soil macroorganisms	LC50 (*Eisenia fetida*, 14 days): >1,000 ppm (OECD Guideline 207) Klimisch score: 1	[1]
PNEC (fresh water)	3.7 µg/L (Assessment factor: 1,000)	
PNEC (marine water	0.37 µg/L (Assessment factor: 10,000)	
PNEC (fresh water sediment)	1.49 mg/kg sediment dw	
PNEC (marine water sediment)	0.149 mg/kg sediment dw	
PNEC (soil)	1 mg/kg soil dw (Assessment factor: 1,000)	

Environmental fate

Bioconcentration factor (BCF)	log BCF: 2.24 (EPISUITE v4.0 BCFBAF v3.00) (QSAR) Klimisch score: 2	[13]
Ready biodegradability	Readily biodegradable (EU Method C.4-C) Klimisch score: 1	[1]
Adsorption/desorption	log K_{OC}: 3.6, 20°C (OECD Guideline 121) Klimisch score: 1	[1]

PBT

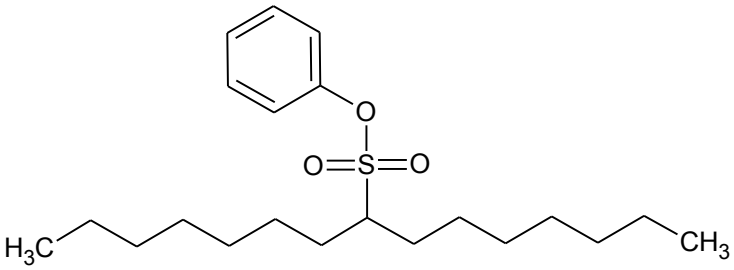
REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Neg; B: Neg; T: Pos; BCF: 170 Fish ChV (mg/L): 0.19 Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 0.46

QSAR bioavailability

Lipinski	Bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	106 metabolites formed. Of these: 106 bioavailable and 0 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	11 metabolites formed. Of these: 11 bioavailable and 0 not-bioavailable. Monoesters formed.
Skin metabolism	18 metabolites formed. Of these: 18 bioavailable and 0 not-bioavailable. Monoesters formed.

Sulfonic acids, C10-21-alkane, Ph esters (ASE)

Identification of substance

CAS No.	91082-17-6
EINECS No.	293-728-5
IUPAC name	Sulfonic acids, C10-C21-alkane, Ph-esters
Structure	
SMILES	O=S(=O)(Oc1ccccc1)C(CCCCCCC)CCCCCCC

REACH

Registration	Full
Submission	Individual submission
Total tonnage	10,000-100,000 tonnes per annum
Harmonised classification	
Notified classification	
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	- g/mole	
Vapour pressure	0.000294 Pa, 20°C (OECD Guideline 104) Klimisch score: 1	[1]
Henry's law constant	0.04-0.061 Pa m³/mol, 20°C (Henry's law constant (HLC) is directly calculated as a ratio of the vapour pressure to the water solubility) Klimisch score: 2	[2]
Water solubility	2.2 mg/L, 20°C (OECD Guideline 105) Klimisch score: 1	[1]
Log K_{OW}	5.7-11.3, 40°C (OECD Guideline 117) Klimisch score: 1	[1]

Ecotoxicological data

Algae	EC0 (*Desmodesmus subspicatus*, 72 hours): >=2 mg/L (EU Method C.3 (Algal Inhibition test)) Klimisch score: 1	[1]
Crustaceans	EC0 (*Daphnia magna*, 48 hours): >=100 mg/L* (EU Method C.2 (Acute Toxicity for Daphnia)) Klimisch score: 1 -	[1]
Fish	LC0 (*Danio rerio*, 96 hours): >=2 mg/L (EU Method C.1 (Acute Toxicity for Fish)) Klimisch score: 1 -	[1]
Terrestrial plants	-	
Soil macroorganisms	-	
PNEC (fresh water)	0.002 mg/L (Assessment factor: 1000)	
PNEC (marine water	0.0002 mg/L (Assessment factor: 10000)	
PNEC (fresh water sediment)	10.03 mg/kg sediment dw	
PNEC (marine water sediment)	1 mg/kg sediment dw	
PNEC (soil)	2 mg/kg soil dw (Assessment factor: -)	

Environmental fate

Bioconcentration factor (BCF)	7-212 (-) Klimisch score: 1	[1]
Ready biodegradability	C10-21-alkane, Ph esters is not readily biodegradable, but is degradable as the pass level of 60 % degradation (BOD) was achieved after 47 days (EU Method C.4-D) Klimisch score: 1	[1]
Adsorption/desorption	log K_{OC}: 4.5-9.3 (PCKOC and other calculation methods) Klimisch score: 2	[2]

PBT

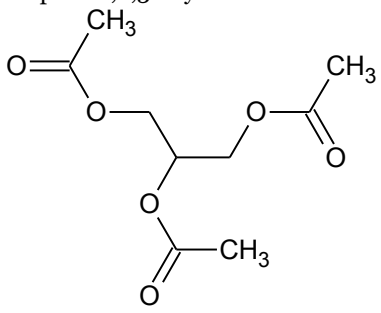
REACH registration dossier	-
QSAR	P: Neg; B: Pos; T: ??; BCF: 790 Fish ChV (mg/L): ?? Half-life (Water, days): 38 Half-life (Soil, days): 75 Half-life (Sediment, days): 340 Half-life (Air, days): 0.75

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	69 metabolites formed. Of these: 69 bioavailable and 0 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	n.d.
Skin metabolism	2 metabolites formed. Of these: 2 bioavailable and 0 not-bioavailable. Monoesters formed.

Triacetin (GTA)

Identification of substance

CAS No.	102-76-1
EINECS No.	203-051-9
IUPAC name	Propane-1,2,3-triyl triacetate
Structure	
SMILES	O=C(OCC(OC(=O)C)COC(=O)C)C

REACH

Registration	Full
Submission	Joint submission
Total tonnage	10,000-100,000 tonnes per annum
Harmonised classification	
Notified classification	
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	218.21 g/mole	
Vapour pressure	0.3306 Pa, 25°C (National Library of Medicine (NLM) http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB) Klimisch score: 2	[1]
Henry's law constant	0.000177 Pa m³/mol, 25°C (HENRYWIN programme v3.20) (QSAR) Klimisch score: 2	[8]
Water solubility	58 g/L, 25°C (National Library of Medicine (NLM) http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB) Klimisch score: 2	[1]
Log K_{OW}	0.25 (National Library of Medicine (NLM) http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB) Klimisch score: 2	[1]

Ecotoxicological data

Algae	EC50 (*Selenastrum capricornutum*, 72 hours): >940 mg/L (OECD Guideline 201) Klimisch score: 1	[1]
Crustaceans	EC50 (*Daphnia magna*, 48 hours): 380 mg/L (EU Method C.2) Klimisch score: 2	[1]
	NOEC (*Daphnia magna*, 21 days): >= 94 mg/L (OECD Guideline 211) Klimisch score: 1	[1]
Fish	LC50 (*Oryzias latipes*, 96 hours): >100 mg/L (OECD Guideline 203) Klimisch score: 1	[1]
	LOEC (*Medaka; Oryzias latipes*, 14 days): (LOEC (14 days, Medaka; Oryzias latipes): 100 mg/) Klimisch score:	[14]
Terrestrial plants	-	
Soil macroorganisms	-	
PNEC (fresh water)	1.88 mg/L (Assessment factor: 50)	
PNEC (marine water	0.188 mg/L (Assessment factor: 500)	
PNEC (fresh water sediment)	4.73 mg/kg sediment dw	
PNEC (marine water sediment)	0.47 mg/kg sediment dw	
PNEC (soil)	0.57 mg/kg soil dw (Assessment factor: -)	

Environmental fate

Bioconcentration factor (BCF)	-	
Ready biodegradability	Readily biodegradable (OECD Guideline 301 B) Klimisch score: 2	[1]
Adsorption/desorption	log K_{OC}: 0.93 (EPIWIN) (QSAR) Klimisch score: 2	[8]

PBT

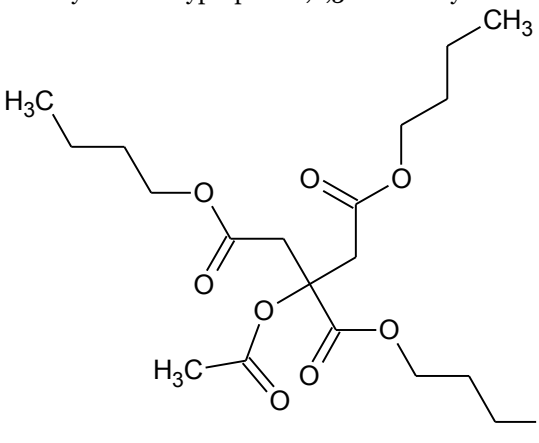
REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Neg; B: Neg; T: Neg; BCF: 3.2 Fish ChV (mg/L): 28 Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 1.9

QSAR bioavailability

Lipinski	Bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	12 metabolites formed. Of these: 12 bioavailable and 0 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	n.d.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	8 metabolites formed. Of these: 8 bioavailable and 0 not-bioavailable. Monoesters formed.
Skin metabolism	3 metabolites formed. Of these: 3 bioavailable and 0 not-bioavailable. Monoesters formed.

Tributyl O-acetylcitrate (ATBC)

Identification of substance

CAS No.	77-90-7
EINECS No.	201-067-0
IUPAC name	Tributyl 2-acetoxypropane-1,2,3-tricarboxylate
Structure	
SMILES	O=C(OC(C(=O)OCCCC)(CC(=O)OCCCC)CC(=O)OCCCC)C

REACH

Registration	Full
Submission	Joint submission
Total tonnage	1,000-10,000 tonnes per annum
Harmonised classification	
Notified classification	Not classified (1286);
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	No
Wide dispersive service life opened/closed	No
Wide dispersive service life closed	No

Physico-chemical characteristics

Molecular weight	402.49 g/mole	
Vapour pressure	0.0494 Pa, 25°C (EPISUITE 4.00 (MPBPVP v1.43), Modified Grain method) Klimisch score: 2	[2]
Henry's law constant	4.434 Pa m³/mol, 25°C (EPIWIN (v4.0), HENRYWIN (v 3.20)) Klimisch score: 2	[2]
Water solubility	4.49 mg/L, 20°C, pH 6.7-6.8 (EU Method A.6 (Water Solubility)) Klimisch score: 1	[1]
Log K_{OW}	4.86, 40°C, pH 7.1 (EPA OPPTS 830.7570) Klimisch score: 1	[1]

Ecotoxicological data

Algae	EC50 (*Desmodesmus subspicatus*, 72 hours): 74.4 mg/L* (OECD Guideline 201) Klimisch score: 1	[1]
Crustaceans	EC50 (*Daphnia magna*, 24 hours): >1 mg/L (OECD Guideline 202) Klimisch score: 2	[1]
	NOEC (*Daphnia magna*, 21 days): >=1.11 mg/L (EU Method C.20 (Daphnia magna Reproduction Test)) (WOE) Klimisch score: 1	[16]
Fish	LC50 (*Lepomis macrochirus*, 96 hours): >38 and <60 mg/L* (OECD Guideline 203) Klimisch score: 2	[1]
	-	
Terrestrial plants	-	
Soil macroorganisms	-	
PNEC (fresh water)	0.022 mg/L (Assessment factor: 50)	
PNEC (marine water	0.0022 mg/L (Assessment factor: 500)	
PNEC (fresh water sediment)	41.5 mg/kg sediment dw	
PNEC (marine water sediment)	4.15 mg/kg sediment dw	
PNEC (soil)	8.29 mg/kg soil dw (Assessment factor: -)	

Environmental fate

Bioconcentration factor (BCF)	31.57 (BCFBAFProgram (v 3.00)) Klimisch score: 2	[2]
Ready biodegradability	Inherently biodegradable Klimisch score: 2	[1]
Adsorption/desorption	log K_{OC}: 4.271 (OECD Guideline 121) Klimisch score: 1	[1]

PBT

REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Neg; B: Neg; T: Pos; BCF: 13 Fish ChV (mg/L): 0.12 Half-life (Water, days): 8.7 Half-life (Soil, days): 17 Half-life (Sediment, days): 78 Half-life (Air, days): 1.1

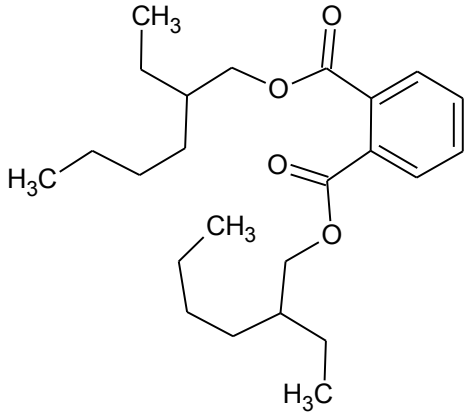
QSAR bioavailability

Lipinski	Bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	n.d.
Microbial metabolism (simulated)	41 metabolites formed. Of these: 40 bioavailable and 1 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	5 metabolites formed. Of these: 5 bioavailable and 0 not-bioavailable. Monoesters formed.
Rat In vivo metabolism(simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	11 metabolites formed. Of these: 11 bioavailable and 0 not-bioavailable. Monoesters formed.
Skin metabolism	21 metabolites formed. Of these: 21 bioavailable and 0 not-bioavailable. Monoesters formed.

Bilag D: Environmental profile of DEHP

DEHP

Identification of substance

CAS No.	117-81-7
EINECS No.	204-211-0
IUPAC name	-
Structure	
SMILES	O=C(OCC(CCCC)CC)c(c(ccc1)C(=O)OCC(CCCC)CC)c1

REACH

Registration	
Submission	
Total tonnage	100,000-1,000,000 tonnes per annum
Harmonised classification	Repr. 1B H360FD
Notified classification	
Wide dispersive end use opened/closed	Yes
Wide dispersive end use closed	Yes
Wide dispersive service life opened/closed	Yes
Wide dispersive service life closed	Yes

Physico-chemical characteristics

Molecular weight	390.56 g/mole	
Vapour pressure	0.0016 Pa, 25°C (US EPA Proposed rules: Vapour pressure. Fed. Reg. 45: 77345-77350, 1980) Klimisch score: 2	[3]
Henry's law constant	-	
Water solubility	0.003 mg/L , 20°C, pH 7 (-) Klimisch score: 2	[1]
Log Kow	7.66 (SPARC v4.5) Klimisch score: 2	[4]

Ecotoxicological data

Algae	EC50 (*Pseudokirchnerella subcapitata*, 72 hours): >0.003 mg/L (OECD Guideline 201) Klimisch score: 2	[1]
Crustaceans	EC0 (*Daphnia magna*, 48 hours): 101.8-165.65 µg/L* (DIN 38412 Tl. 11) Klimisch score: 2	[3]
	NOEC (*Daphnia magna*, 21 days): 0.158 mg/L* (OECD Guideline 211) Klimisch score: 2	[1]
Fish	LC50 (*Fathead minnow*, 96 hours): >0.16 mg/L* (US EPA-660/3-75-009, method for acute toxicity tests with fish, macroinvertebrates, and amphibians. 1975) Klimisch score: 2	[1]
	NOEC (*Oryzias latipes*, 90 days): 5,000 µg/L* (no guideline followed) Klimisch score: 2	[2]
Terrestrial plants	NOEC (*Triticum aestivum/Lepidum sativum/Brassica alba*, 18 days): 100 mg/kg soil dw (OECD Guideline 208) Klimisch score: 1	[1]
Soil macroorganisms	LC50 (*Eisenia fetida*, 7 days): >1,000 mg/kg soil dw (OECD Guideline 207) Klimisch score: 1	[1]
PNEC (fresh water)		
PNEC (marine water		
PNEC (fresh water sediment)	100 mg/kg sediment dw (Assessment factor: 10)	
PNEC (marine water sediment)	20 mg/kg sediment dw (Assessment factor: 50)	
PNEC (soil)	13 mg/kg soil dw (Assessment factor: 10)	

Environmental fate

Bioconcentration factor (BCF)	1,380 (no guideline followed) Klimisch score: 2	[1]
Ready biodegradability	readily biodegradable (EU Method C.4-C Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) Klimisch score: 1	[1]
Adsorption/desorption	log K_{OC}: 5.68 (EPA OTS 796.2750 Sediment and Soil Adsorption Isotherm) Klimisch score: 2	[1]

PBT

REACH registration dossier	The substance is not PBT / vPvB
QSAR	P: Neg; B: Neg; T: ??; BCF: 1,700 Fish ChV (mg/L): ?? Half-life (Water, days): 15 Half-life (Soil, days): 30 Half-life (Sediment, days): 140 Half-life (Air, days): 0.75

QSAR bioavailability

Lipinski	Not bioavailable
Mammalian metabolism	
Microbial metabolism (observed)	4 metabolites formed. Of these: 4 bioavailable and 0 not-bioavailable. Monoesters formed.
Microbial metabolism (simulated)	62 metabolites formed. Of these: 51 bioavailable and 11 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (observed)	2 metabolites formed. Of these: 2 bioavailable and 0 not-bioavailable. Monoesters formed.
Rat In vivo metabolism (simulated)	
Rat Liver S9 metabolism (observed)	n.d.
Rat Liver S9 metabolism (simulated)	5 metabolites formed. Of these: 5 bioavailable and 0 not-bioavailable. Monoesters formed.
Skin metabolism	14 metabolites formed. Of these: 10 bioavailable and 4 not-bioavailable. Monoesters formed.

Environmental Impacts Of Certain Phthalates And Alternatives To Phthalates

The report gives an overview of the environmental effects of 28 phthalates and 10 non-phthalates all potential alternative plasticisers to the 4 classified phthalates (DEHP, DBP, BBP and DiBP). Data have been compiled from the REACH registration dossiers and certain databases. The conclusion is that the alternatives do not show more negative effects to the environment than the 4 classified phthalates, but it has to be recognized that the data in some cases are limited.

Rapporten giver et overblik over miljøeffekterne af 28 ftalater og 10 ikke-ftalater, som alle er potentielle alternative blødgørere til de 4 klassificerede ftalater (DEHP, DBP, BBP og DIBP). Data er indsamlet fra REACH registreringsdossiers og visse databaser. Konklusionen er, at alternativerne ikke viser mere negative virkninger for miljøet end de 4 klassificerede ftalater, men datamængden er i nogle tilfælde begrænset.

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