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Identifying potential POP and PBT substances

Development of a new Persistence/ Bioaccumulation score

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Abstract

Identifying potential POP and PBT candidates

Development of a new Persistence/Bioaccumulation score

RIVM has screened the potential for long-term fate in the environment of a large number of substances. For this purpose a new methodology has been developed which indicates whether substances will persist in the environment and/or bioaccumulate in biological organisms. The results are a first step towards selection of substances which have inherent chemical properties that potentially make them a long-term hazard for the environment.

Further research into the actual persistence and bioaccumulation of these substances in the environment will be needed. This information is necessary for proposing selected substances under REACH as Persistent, Bioaccumulative and Toxic substances (PBTs) or very Persistent and very Bioaccumulative substances (vPvBs), or when they are proposed within the Stockholm Convention as Persistent Organic Pollutants (POPs). Once identified as PBT, vPvB or POP, further risk management measures or even a ban on production and use of such chemicals may follow. REACH (Registration, Evaluation and Authorization of Chemicals) is the European chemical substances regulation, in force since June 2007, which aims to evaluate and minimize all risks of chemicals produced and/or used in the European Union. The international Convention of Stockholm, in force since May 2004, aims to minimize or eliminate the presence of POPs in the world.

In many cases, the harmful potential of substances that were later identified as POPs and PBTs only became apparent after scientists were alarmed by monitoring results looking for these substances in the environment. Nowadays, most new substances are screened on potential long term hazard to the environment before they are introduced to the market. However, for a large number of existing substances on the (European) market their potential hazard has never been evaluated, since such an evaluation was not required in the past, or because their market volumes were so small. The Persistence/Bioaccumulation score presented in this report can be used as a tool to quickly screen data-poor substances for their potential environmental persistence and bioaccumulation in the food chain.

Keywords:
PBT candidates, POP candidates, REACH, Stockholm Convention

Rapport in het kort

Identificatie van potentiële POP- en PBT-stoffen

Ontwikkeling van een nieuwe score voor Persistentie en Bioaccumulatie-potentieel

Het RIVM heeft van een zeer groot aantal stoffen de schadelijkheid bekeken. Hiervoor is een methodiek ontwikkeld waarmee kan worden onderzocht in welke mate deze stoffen in het milieu worden afgebroken dan wel zich in organismen ophopen. De resultaten zijn een eerste stap om stoffen te selecteren die vanwege hun chemische karakter gevaarlijk lijken te zijn.

Nader onderzoek zal nodig zijn naar de mate waarin deze stoffen in de praktijk afbreken en/of ophopen. Deze informatie is nodig om geselecteerde stoffen via de REACH-verordening of het Stockholm-verdrag voor te kunnen dragen als Persistente Bioaccumulerende en Toxische (PBT) stoffen en Persistente Organische Verbindingen (POP). Als stoffen eenmaal aangemerkt zijn als POP en/of PBT zal dat leiden tot beperkingen of een verbod op de productie en het gebruik van deze stoffen. REACH (Registration, Evaluation and Authorisation of CHemicals) is de Europese wetgeving voor gevaarlijke stoffen die sinds 2007 van kracht is om de risico's van chemische stoffen in kaart te brengen en te beperken. Het internationale Verdrag van Stockholm, dat in werking trad in mei 2004, streeft ernaar de aanwezigheid van POP's in de wereld te elimineren of te beperken.

In veel gevallen is de schadelijkheid van stoffen die later als POP en/of PBT zijn aangemerkt pas aan het licht gekomen nadat wetenschappers gealarmeerd werden door onderzoeksresultaten van monitoring studies van deze stoffen. Tegenwoordig wordt van de meeste stoffen standaard bekeken hoe schadelijk ze zijn voordat ze op de markt worden gebracht. Van een groot aantal stoffen is de schadelijkheid echter nog niet vastgesteld, omdat in het verleden minder strenge eisen werden gesteld toen ze op de markt werden gebracht, of omdat het om zeer beperkte marktvolumes gaat. De nieuw ontwikkelde Persistentie en Bioaccumulatie Score, zoals gepresenteerd in dit rapport, kan een belangrijke rol spelen in een snelle screening van deze stoffen waarvan nog weinig of geen gegevens bekend zijn.

Trefwoorden:
PBT kandidaten, POP kandidaten, REACH, Stockholm Conventie

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Summary

In this report, a new methodology for the calculation of potential environmental persistence and bioaccumulation in the food chain is presented. This so called PB-score is based completely on theoretical properties derived from the chemical structure, so no experimental data are needed as input. This allows for the rapid calculation and subsequent comparison of the (calculated) P- and B-properties of thousands of substances, making it an ideal tool for quick screening and prioritizing exercises.

The need for such screening and prioritizing work comes from, amongst others, the wish to generate working lists of proposed substances for regulation in international frameworks like REACH (PBT and vPvB substances) and the Stockholm Convention (POPs). Instead of ranking (reorganizing lists in order of priority) or binning (labelling groups of substances with an equal level of concern) we proposed a quantitative, continuous score which would also allow expressing a relative level of concern when compared to other substances, e.g. existing POPs and confirmed PBT/vPvB substances.

The resulting PB-scores (and its components the P- and B-scores) have been calculated for 64.721 substances coming from different lists of substances which bear commercial relevance. The top-scoring substances from this exercise might form an excellent longlist of potential PBT/vPvB/POP substances which can become candidates for risk management. In order to further substantiate the concern for PB properties in the real world, information on production/import tonnage levels is required first. For the actual proposal of candidates in either REACH or Stockholm Convention frameworks experimental confirmation of the suspected P- and B-properties may also be needed.

Because of the modular structure of the PB-score, adaptation to a specific regulatory framework is possible by adapting the cut-off values used for scaling the scores. Inclusion of an additional Toxicity term (e.g. for REACH PBT assessment) or a Long Range Transportation term (for Stockholm Convention POP candidates) can also be easily accomplished, although this will give rise to (more) discussion on the individual weight of the different terms in an overall score. For the current study only Persistence and Bioaccumulation properties have been combined into a PB-score, with the (calculated) P- and B-properties weighted equally.

The performance of this newly developed PB-score was measured by evaluating the individual scores for the known POP and confirmed EU PBT/vPvB substances. All POPs have been calculated to have high PB-scores, with the exception of the confirmed POP hexabromobiphenyl and the proposed POP trifluralin. In both cases, the calculated B-score would indicate that the formal POP criteria for bioaccumulation are not met based on their calculated properties.

The performance of the PB-score for identifying confirmed PBT and/or vPvB substances is comparable to its performance for known POP substances, with only few substances where the calculated PB-score would indicate no potential PBT (or vPvB) properties. It is also noted in the exercise that there are limitations to the applicability of the theoretically calculated PB-score, as e.g. metallo-organics like tetrabutyl-tin and tetramethyl-lead are incorrectly calculated to have low persistence (tin) or both persistence and bioaccumulation potential (lead). This can be related to the (known) poor performance of the applied (Q)SARs for metallo-organic substances.

The overall conclusion is that the developed PB-score is a highly practical and rapid approach to screening and prioritization, and the generated list of highest scoring substances is thought to contain highly relevant substances which can be used to propose PBT/vPvB and POP candidates.

1 Introduction

Persistent organic pollutants (POPs, section 1.2) and Persistent, Bioaccumulative and Toxic (PBT, section 1.3) substances are priority substances with regard to potential risks to humans and ecosystems. This is due to their characteristics with regard to persistence (P) in the environment, accumulation in biological organisms (bioaccumulation; B), and toxicity (T). POPs and PBT chemicals can potentially give rise to serious human health and environmental effects. Concern about these substances is based on the potential impact that POPs and PBTs can have on a large scale with regard to geography and time, typically over several generation. This concern is increased by the assumption that current quantitative risk assessment procedures would not reflect the complex behaviour of these substances due to release, distribution and redistribution in the environment and subsequent long-term exposure. POPs and PBTs have been found all over the globe in wildlife, food, human breast milk and blood. Examples of typical and well known POP or PBT substances are DDT, PCBs, polychlorinated dibenzo-p-dioxins, brominated flame-retardants, and several chlorinated pesticides.

1.1 Priority Setting

Many chemical substances are currently on the market, and only a limited number of those substances have been evaluated on their PBT and POP characteristics. This is because, until recently, placing new and existing substances on the market did not necessitate a comprehensive investigation of the substance PBT and POP characteristics. Thus, for many of these existing substances it is not known if they potentially fulfil the criteria for being considered a POP or PBT chemical.

In general, adding a substance to the list of one of the POP/PBT protocols or regulations, requires that a comprehensive dossier of the substance is being compiled, containing data on the physical-chemical characteristics of the substance, its production and use, its toxicological properties etc. Collecting sufficient data (including modelling data as well as monitoring data) is very time and money consuming, which makes it almost impossible to deal with all existing substances short-term. However, the parties involved in the various Conventions, Protocols and Regulations have a high interest in knowing if there are new POP/PBT candidates currently on the market, which may lead to exposure and risks for man and environment, and consequently would need regulation as soon as possible.

1.2 POP regulations

Historically, two different policy fields have been involved with Persistent Organic Pollutants (POPs) in the environment (i.e. air quality and chemical safety), and within each field an international convention on POPs was formulated. Firstly, under the auspices of the United Nations Economic Commission for Europe (UNECE), the international community on air quality recognized the potential hazards of POPs, which resulted in a specific POP Protocol under the Convention on Long-range Transboundary Air Pollution [UN-ECE, 1996]. This UNECE POP Protocol encourages the research, emission reduction and monitoring of POPs, as well as the international co-operation between scientists. Secondly, the United Nations Environment Programme [UNEP, 1995], which focuses on chemical safety, described its policy on POPs in the Stockholm Convention [UNEP, 2001]. At present, November 2010, 29 parties have ratified the UNECE POP Protocol to the Convention on Long-range Transboundary Air Pollution (LRTAP Convention) and 146 parties have ratified the Stockholm Convention.

At the start of the Convention, a set of substances, or groups of substances, was identified within the Stockholm Convention and the UNECE Protocol on POPs as a first set of POPs. Since then, new POPs have been added to both conventions. The presently adopted substances are given in Table 1.

Table 1 POPs identified within the UNEP Stockholm Convention[b] and/or the UNECE Protocol[c] (as of December 2010)

Organochlorine pesticides	**Industrial chemicals**	**Unintentional byproducts**
Aldrin	Hexachlorobenzene (HCB)[a]	Hexachlorobenzene (HCB)[a]
Chlordane	Polychlorinated biphenyls (PCBs)[a]	Polychlorinated biphenyls (PCBs)[a]
Chlordecone	Pentachlorobenzene[a]	Pentachlorobenzene[a]
DDT	Hexabromobiphenyl	Polychlorinated dibenzodioxins (PCDDs)
Dieldrin	Octabromodiphenyl ether (OctaBDE)[b]	Polychlorinated dibenzofurans (PCDFs)
Endrin	Pentabromodiphenyl ether (PentaBDE)[b]	Polycyclic aromatic hydrocarbons (PAHs)[c]
Heptachlor	Perfluorooctane sulfonic acid (PFOA), its salts, and perfluorooctanesulfonylfluoride	α-HCH[a,b]
Mirex		β-HCH[a,b]
Toxaphene		
Pentachlorobenzene[a,b]		
Hexachlorobenzene (HCB)[a]		
Hexachlorocyclohexane (HCH, techn.)[c]		
Lindane (γ-HCH[b]), α-HCH[a,b], β-HCH[a,b]		

[a] Pentachlorobenzene, α-HCH, β-HCH, PCBs and HCB are listed simultaneously as organochlorine pesticide, industrial chemical and/or unintentional byproduct.

[b] α-HCH, β-HCH, commercial octa- and penta-BDE, lindane and pentachlorobenzene are only listed under the UNEP Stockholm Convention. The meaning of OctaBDE and PentaBDE in the Stockholm convention is further elaborated in section 3.2.3 and in the footnotes to Table 9.

[c] HCH (techn.) and PAHs are only listed under the UNECE POP Protocol

Under both conventions, a mechanism exists for the identification and inclusion of additional POPs. Parties to both Conventions may submit proposals for listing a chemical in one of the annexes to the conventions. If the proposal contains the necessary information it will be discussed by a scientific committee (POP Review Committee and Task Force POP respectively), which will apply the screening criteria. When the criteria are met, the substance is processed further. Although the processes differ slightly between both conventions, they are characterized by a stage in which the risk profile for the chemical is discussed and one in which risk management is evaluated. A final decision if the substance should be considered as a POP is being made by the Conference of Parties under the Stockholm Convention or the Executive Body under the LRTAP Convention on the basis of the recommendations of the POP Review Committee and Task Force POP respectively.
The process of nomination takes several years and starts with the nomination dossier which contains literature data on the screening criteria (P, B, T and LRTAP), data on production and use, data supporting the likelihood of adverse effects and legislation. The presence of literature data is crucial in the nomination process, although the Stockholm Convention also states that lack of full scientific certainty shall not prevent the proposal from proceeding. Several substances have currently been under consideration for inclusion in one or both conventions, e.g. perfluorooctanesulfonate (PFOS), pentabromo diphenyl ether (PeBDE) and pentachlorobenzene [Scheringer, 2009].

1.3 PBT regulations

The European Union, the United States, Canada, and several other countries have legislation in place to identify and regulate current-use of commercial PBT substances under their jurisdictions. The PBTs that are identified in this way can be put forward as candidates for consideration in the POP regulations as described in section 1.2.

In the United States, PBT substances can be identified under the Toxic Substances Control Act (TSCA), which is currently being revised. The EPA screens substances that are new to the market for PBT characteristics, and can ask for additional information on PBT characteristics. This can be done in the case of potential risk of injury to human health or the environment, if the substance will be produced in substantial quantities and if there may be significant or substantial human exposure to the substance or if the substance is anticipated to enter the environment in substantial quantities. How to improve the control of PBT substances under the TSCA act is currently being debated [US Subcommittee on Commerce, Trade, and Consumer Protection, 2010].

In Canada, a categorization of substances on the domestic substances list (DSL) was undertaken according to the provisions of the Canadian Environmental Protection Act [CEPA, 1999]. About 400 substances on the DSL are considered to be potential PBTs and according to the Canadian criteria, are designated as Persistent, Bioaccumulative and inherently Toxic (PBiT)) to non-human organisms [Environment Canada, 2006]. Many of these substances, however, are currently not being marketed in Canada.

In Europe, PBTs are mentioned in various types of legislation, such as those for biocides, pesticides, (veterinary) medicines, and the production and marketing of industrial substances (REACH) [EU, 2006]. PBTs are further mentioned in the Water Framework Directive and in the OSPAR Convention. Except for OSPAR [OSPAR 2005], the criteria for identification of PBTs in all these legislative frameworks are similar to those defined in Annex XIII of REACH [EU, 2006][1].
Identification of a substance as a PBT substance or a very persistent, very bioaccumulative (vPvB) substance is possible in all the above-mentioned frameworks, as well as in the Stockholm Convention and the UNECE Protocol on POPs. The REACH Regulation is a legislation where producers or importers of PBT/vPvB substances have specific obligations regarding these substances. As part of the registration procedure in REACH, every substance that is registered needs to be screened for PBT/vPvB properties as part of the Chemical Safety Assessment (substances manufactured or imported in volumes > 10 tpa). If a substance is recognized as a PBT/vPvB in the registration dossier, strict emission controls are triggered in order to minimize emission and subsequent exposure to PBT/vPvB substances. In addition, PBT and vPvB substances can be made subject to the authorization regime of REACH. The authorization provisions require those using or making available substances of very high concern, such as PBTs and vPvBs, to apply for an authorization for each use. Applicants for authorization of PBTs/vPvBs should demonstrate that the socio-economic benefits outweigh the risks by submitting a substitution plan along with a socio-economic analysis.
Authorization is required for substances included in Annex XIV of REACH. A procedure exists enabling EU member states or the EU Commission to submit a so-called Annex

[1] Following a review a review of the criteria in Annex XIII, the Commission concluded that an adaptation of the criteria for the identification of PBT and vPvB substances is necessary. The Commission has consulted the REACH Competent Authorities and stakeholders. A Commission Regulation amending Annex XIII is expected in 2011. Under the Commission's new procedure, "all available information is to be considered and will be used in a so-called 'weight of evidence approach".

XV dossier that identifies a substance as a PBT/vPvB according to the REACH criteria. If the PBT/vPvB status is accepted by the European Chemicals Agency (ECHA) in conjunction with the Member State Committee (MSC), the substance is added to the candidate list for inclusion in Annex XIV of REACH. At the moment of writing, the candidate list contains 9 PBT/vPvB substances [ECHA 2010]. In an additional procedure, the substance can be prioritized for inclusion in Annex XIV, which involves ECHA, the MSC and final adoption by comitology decision, and publication by the European Commission and the Parliament. Of the substances included in the candidate list, ECHA recommended on the 1st of June 2009 that musk xylene, HBCDD and SCCPs should be placed on Annex XIV, which was adopted by comitology in Autumn 2010.

1.4 POP and PBT (screening) criteria

The Stockholm Convention, the UNECE POP Protocol under the LRTAP Convention and REACH (PBTs) contain screening criteria or indicative values to identify potential POPs/PBTs. In later phases of the nomination process, e.g in drafting the risk profile, these values are also used. Both POP frameworks focus on long-range transport, persistency and bioaccumulation. Toxicity is not described by clear-cut criteria, but is rather described as reason for concern or as 'toxicity or ecotoxicity data that indicate the potential for damage to human health or to the environment'. By contrast, the REACH PBT definition gives clear toxicity criteria for PBT substances, but also introduces a category of vPvB substances (with stricter P- and B-criteria), where toxicity is not a criterion. These criteria are summarized in Table 2.

1.5 Previous studies on POP/PBT selection or prioritization

Searching for potential new POP and PBT substances is not new; in the past, a number of studies were performed in order to select chemical substances as potential new POPs and PBTs. Similar studies are known from BKH consultants [Blok 1997], COMMPS/WFD [Klein 1999], Michigan State University [Snyder, 2000], the Danish EPA [Tyle 2002] the Swedish EPA/KemI [KemI/EPA 2002], OSPAR [OSPAR, 2006], and the PBT profiler as developed by the USEPA [EPA 2008]. The outcomes of these studies, as well as the methodologies applied are considered relevant as a starting point for this study. A detailed description of these studies is given in Appendix I of this report.

Although it is considered very useful to review these studies and compare them with the findings of the current study, most of them differ significantly from the present study in set-up and/or in the group of substances accounted for. A significantly smaller base set of chemical substances has been reviewed by the Swedish EPA/KemI, by OSPAR and in the COMMPS procedure. Moreover, OSPAR focused on the marine environment while COMMPS centred on the fresh water environment. As a result, the POP criteria employed in these studies were not fully in agreement with those under the Stockholm Convention and the UNECE POP Protocol. Besides, production amounts reported in the OSPAR reports might be outdated. The procedure used by Michigan State University combines theoretical and experimental data and focuses on uncertainties in the data, with the aim of ranking substances for prioritization. The various studies also applied different procedures: the COMMPS procedure, for example, was based on rankings of substances instead of on rigid criteria, whereas BKH consulting applied the availability of toxicity data as a first criterion to select potential PBTs, thereby neglecting a large group of compounds for which no toxicity data were then available.

The results of the study of the Danish EPA could be considered most compatible with the approach followed in this study, due to the consistency in the criteria applied for

identification of POP/PBT-like substances. However, that study deviates from the current study on four counts:

1) In the study of the Danish EPA, no environmental fate modelling was incorporated. In the procedure as proposed in this study, rather than the half-life of substances in single isolated compartments, , but rather the overall persistence in the environment was used as indicator for persistency, taking into account degradation in all compartments and redistribution between the compartments, including (long-range) transport.
2) The quantitative structure-activity relationship (QSARs) applied for estimating bioaccumulation potential in the Danish study did not account for metabolism, nor was there an assessment of the biomagnification potential in air-breathing organisms.
3) The study of the Danish EPA starts with a large base set of data (all organics from the EINECS list), but compared to the present study, pesticides, biocides and pharmaceuticals that are not on EINECS were not considered. Around 50.000 substances were evaluated in the Danish exercise where the present study increases this number to a total of almost 65.000.
4) A good aspect of the study of the Danish EPA is the attention that is paid to the toxic properties of substances. The toxicity endpoint has not (yet) been considered in the current study.

1.6 Aim of the current study

The goals of the current study are to develop a methodology through which substances can be evaluated concerning their PBT and POP characteristics, to perform a screening assessment with a large set of existing chemical substances and to identify those substances that show the most POP- or PBT-like properties.
The final aim is to compose a list of prioritized substances which can be used in the (near) future for more in-depth assessments to identify actual POP or PBT/vPvB characteristics, and the corresponding follow-up actions that could include the preparation of actual dossiers for formal review of the identification of the PBT, vPvB or POP status. Although the report focuses mainly on POP and vPvB substances, substances fulfilling the P and B criteria can also be identified by means of this methodology (for criteria, see Table 2).

Table 2 UNECE and UNEP POP and EU PBT/vPvB Criteria
(also see footnote on page 13)

criteria	UNEP/UNECE POP	EU PBT	EU vPvB
Potential long-range environmental transport	• Atmospheric t½ > 2 days and P < 1000 Pa • Measured levels in remote areas or via migratory species, air or water	• no criterion	• no criterion
Persistence	• Water: t½ > 2 months or • Soil: t½ > 6 months or • Sediment: t½ > 6 months or • Other evidence	• Fresh or estuarine surface water: t½ > 40 days, or • Marine surface water: t½ > 60 days, or • Soil or fresh or estuarine water sediment: t½ > 120 days or • Marine sediment: t½ > 180 days	• Marine, fresh, or estuarine surface water: t½ > 60 days or • Soil, or marine, fresh or estuarine water sediment: t½ > 180 days
Bioaccumulation	• BCF > 5000 or log K_{ow} > 5 • Other, e.g. very toxic • Monitoring data	• aquatic organisms BCF > 2000 or log K_{ow} > 4.5	• aquatic organisms BCF > 5000 or log K_{ow} > 4.5
Toxicity	• Reasons for concern • Evidence of adverse effects • Toxicity or ecotoxicity data that indicate the potential for damage	• Chronic NOEC for marine of freshwater organisms < 0.01 mg/l or • Classified* as carcinogenic (cat.1 or 2), mutagenic (cat.1 or 2), or toxic for reproduction (cat.1, 2 or 3) or • Chronic toxicity indicated by T, R48* or Xn, R48*	• no criterion

* EU Classification and Labelling according to Directive 67/548/EEC

2 Materials and methods

2.1 Approaches to prioritization

In selecting potential PBT and POP substances, a stepwise approach on the basis of the hazard characteristics of the various substances was followed. Lists of substances from various backgrounds, such as industrial substances, pesticides and pharmaceuticals, were combined to create a long list of substances. Where possible, these substances were characterized by CAS number and chemical structure information. The chemical structure information was used to generate characteristics on persistence, bioaccumulation, long-range transport and toxicity using theoretical models (QSARs). To be able to cover as many substances as possible, QSAR estimates were used instead of experimental data. Because no reliable estimates for toxicity could be generated for this large number of substances, the exercise is in first instance restricted to persistence and bioaccumulation. In the course of this study, three approaches were examined to prioritize substances based on the calculated properties: binning, ranking and scoring.

Binning

The most straightforward approach is to bin the substances into categories, for example a category fulfilling the screening criteria for POP, the criteria for PBT or not. The EPA PBT profiler is an example of a tool, which uses three bins (green, orange and red) to indicate whether a substance fulfils the (EPA specific) criteria for PBT substances or not. The big advantage of the binning approach is its simplicity and ease of interpreting the results. Moreover, it will not create a (possibly false) idea of precision regarding the estimation methods used. This approach, however, has two major disadvantages. Firstly, no distinction between substances in one bin can be made, and if the highest priority bin is filled with a large number of substances, one still needs to somehow further prioritize the substances in this highest priority bin. Secondly, bins are based on a strict division between substances that do fulfil the criteria and those that do not. However, the relationship between the calculated properties and the criteria is not unambiguous, which makes it difficult to filter false positives and false negatives from the large number of substances within each bin.

Ranking

A second approach is sorting substances according to the properties of interest (P, B) and using the subsequently assigned rank as a measure of potency. This means that the most persistent substance is given rank 1, the second most persistent substance is given rank 2 etc., and the same is done for bioaccumulation. The P- and B-rank numbers can easily be added to give a combined PB-ranking. For example: a substance which ranks 100 for its persistence and 50 according to its bioaccumulative properties will get a rank value of 150. The disadvantage of this procedure is that it does not provide information on the actual difference in persistency or bioaccumulation between two substances, i.e. the 'steps' between two subsequent substances always have a value of 1, independent of the actual values for P and B of these two substances. If, for example, the first 1000 substances are all predicted to be non-degradable, any substance that is slightly but not significantly degradable will end up in a ranking beyond 1000. Furthermore, the ranks are always relative to the list of evaluated substances. Therefore, it is not possible to interpret these ranks as absolute values. Before carrying out a more sophisticated method for prioritizing substances based on their P- en B-characteristics, a ranking study was performed. The results of this exercise are recorded in Appendix 3 to this report.

Scoring

To overcome the above-mentioned disadvantages, the predicted measures for persistency and bioaccumulation were converted to scores (P-score and B-score) that range from zero to one. In this way, the very persistent substances ideally will have a P-score close to one, while the readily degradable substances will have a score close to zero and in a similar way the B-score is based on the prediction for bioaccumulation. Because scoring outperforms the other two approaches, this approach was used for the analyses in this report. The way in which the score is calculated is further described in section 2.2.

Although production, use, toxicity and concentration in the environment may be important criteria in the prioritization of substances that are potential POP or PBT candidates, these characteristics were not considered. Screening the selected substances against these characteristics should be considered in a next step. In such a step, the validity of the selected substance in fulfilling the P and B criteria in reality and the relevance should also be evaluated.

2.2 Calculation of a theoretical PB-score

To express the relative amount of concern for Persistence and Bioaccumulation (relative to other substances, or relative to known POPs and/or PBT substances), a quantitative, continuous score is developed, based on properties that can be calculated directly from structure. Separate P- and B-scores are calculated first, which should allow for individual weighting of the P- and B-properties relative to each other. This will also allow adding other properties (e.g. Toxicity or Long Range Transport potential) in a similar manner for future improvement/extension of the PB-score. Initially, the Long Range Transport Potential (LRTP) was planned to be an additional factor in the calculation of a theoretical PB-score, However, the overall Persistence (P_{ov}) used for calculating the P-score already contains persistence in air which is one of the elements within LRTP. During the ranking exercises (Appendix 3), it was observed that taking into account LRTP did not change the order of the highest 250 substances. Still, LRTP can easily be included as part of, e.g., a POP-specific score, by following the same steps as indicated for Persistence (section 2.2.1) and Bioaccumulation (section 2.2.2). Adding LRTP will, however, give rise to discussion on how much weight should be given to this property relative to Persistence and Bioaccumulation.

2.2.1 Persistence

Current regulations use thresholds for individual half-lives in air, water, soil and sediment (see section 2 and Table 2) as criteria for persistency of a substance. If a threshold for half-life in any one of the compartments is exceeded, a substance fulfils the (screening) requirements for classification as a POP and/or PBT substance. However, exceeding the threshold for half-life in a compartment to which a substance will not significantly partition, or a very rapid degradation in other (relevant) compartments might make a substance non-persistent in the environment. In the literature overall persistence, P_{ov}, has been proposed as a measure for chemicals assessment [Stroebe 2004], specifically for the PBT and POP assessments. P_{ov} uses information on both the degradation behaviour and the partitioning behaviour of a substance over different environmental compartments, by coupling individual compartment degradation half-lives with a multimedia fate model. For development of the P-score, the P_{ov} is calculated using the OECD P_{ov}&LRTP screening tool, version 2.1 [OECD 2008].

Overall Persistence – P_{ov}

The OECD P_{ov} and LRTP Screening Tool has been developed with the aim of using multimedia models for estimating overall persistence (P_{ov}) and long-range transport potential (LRTP) of organic chemicals at a screening level, in the context of PBT/POP assessments. The Tool requires estimated degradation half-lives in soil, water and air (t1/2 water, air, soil), and partition coefficients between air and water (K_{aw}) and between octanol and water (K_{ow}) plus the molecular weight (MW) as substance-specific input parameters. From these inputs the Tool calculates P_{ov} as a half-life in days and LRTP as a characteristic travel distance (CTD) in kilometres. The required input is shown in the screenshot from the OECD LRTP and P_{ov} screening tool, presented in Figure 1.

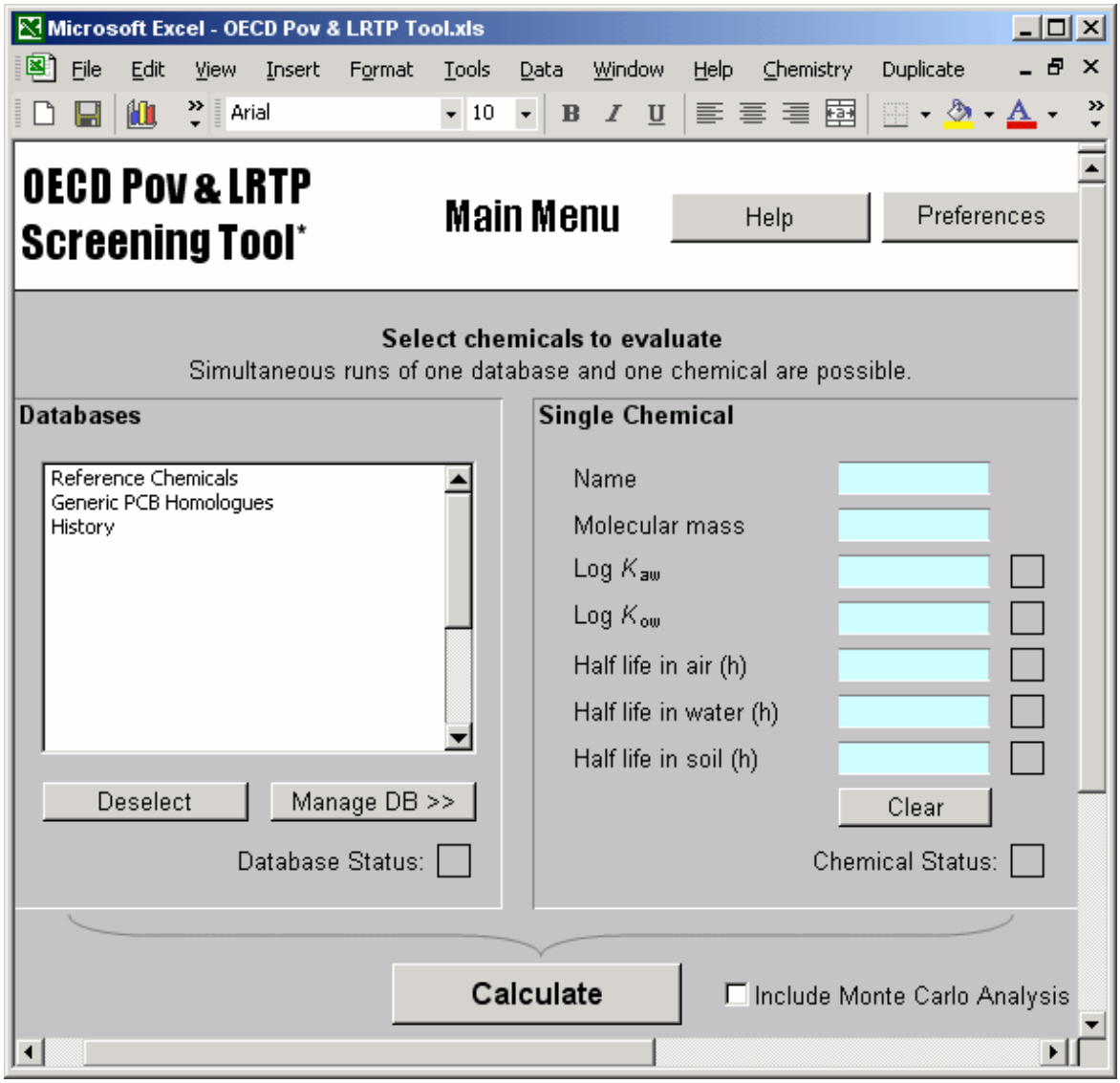


Figure 1. Input screen showing the required parameters (blue cells) for the calculation of the overall Persistence (P_{ov}) using the OECD P_{ov} & LRTP screening tool.

Calculation of the input parameters for P_{ov}

The six parameters required for the estimation of the P_{ov} were all calculated using theoretical (QSAR) models, which (only) require the chemical structure as input.

Molecular Weight

The molecular weight (MW) was directly calculated from the chemical structure assigned to the CAS number (see section 2.3.2).

Octanol-water partition coefficient

The octanol-water partition coefficient K_{ow} was estimated using KowWin v.1.67 as developed by Syracuse Inc. for the US EPA. The methodology is described in Meylan and Howard (1995). The ClogP estimation programme from BioByte Inc. is also frequently mentioned for estimation of log K_{ow}, e.g. in the REACH guidance documents on bioaccumulation. In contrast to KowWin, this software requires a commercial licence, making reproduction of the scores difficult for anyone not having such a licence. Furthermore, the KowWin estimation routine is shown to give better overall statistical performance than the ClogP routine (Meylan & Howard 1994) and also performs best when compared to other log K_{ow} estimation routines (van Leeuwen & Vermeire 2007).

Air-water partition coefficient

The air-water partition coefficient log K_{aw} is used in the environmental fate modelling applied in the OECD P_{ov}&LRTP tool, and for our exercise it was estimated using HenryWin v.3.20 as developed by Syracuse Inc. for the US EPA. HenryWin estimates the Henry's Law Constant (the air-water partition coefficient, K_{aw}) of organic compounds at 25°C using the methodology originally described by Hine and Mookerjee (1975). The original methodology was updated and expanded at Syracuse Research Corporation as described in Meylan and Howard (1995). The octanol-air partition coefficient K_{oa} required for calculation of the trophic magnification factor (TMF, section 2.2.2.2) can be derived by dividing the K_{ow} by the K_{aw}.

$$K_{oa} = \frac{K_{ow}}{K_{aw}}$$

Half-life in water

The half-life in water was estimated using the BIOWIN estimation programme v.4.10. Biodegradability estimates from this programme are based upon fragment constants that were developed using multiple linear or non-linear regression analyses, depending on the specific sub-model. Specifically, the Biowin3 sub-model gives an estimate of the time required for 'complete' ultimate biodegradation in the aquatic environment, as estimated by a panel of experts. This sub-model does not give a direct estimate of half-life, but a value between 1 and 5, which should be interpreted as 5 - hours; 4 - days; 3 - weeks; 2 - months; 1 - longer. It should be noted that the ratings are only semi-quantitative and are not half-lives. Thus, for example, if the average expert rating for ultimate degradation of a compound is 2.5, it means the experts considered that the compound would biodegrade completely in a time frame somewhere between weeks and months, with no exact time or half-life being applied. For our purpose of a continuous, quantitative P-score, however, we do want to interpret this value as a half-life. Aronson et al. (2006) assigned half-lives in surface water to the outcome of the Biowin3 sub-model. This was done using bins with a range of 0.5 units of the Biowin3 values. A continuous function was derived from these data by assigning the half-life for each bin to the average Biowin3 value for

each bin and fitting an exponential function through these points. The resulting function gives us the half-life in water in days:

$$half-life_{water} = 7300 \cdot \exp^{(-2 \cdot BIOWIN3)}$$

For input into the OECD P_{ov}&LRTP screening tool this half-life needs to be multiplied by 24 to give a half-life in hours.

Half-life in soil

No direct estimate of the half-life in soil (or in sediment) could be found. However, it is generally acknowledged that the half-life in soil is related to the half-life in water (Aronson, 2006). Using data presented by Boethling et al. (1995), a factor of 1.85 is calculated as the mean ratio between half-lives in soil and half-lives in water. As a conservative estimate we have used a factor of two:

$$half-life_{soil} = 2 \cdot half-life_{water}$$

Half-life in air

The half-life in air was directly calculated from the estimate of OH-radical reactivity of the substance using the AOPWin v1.92. This programme estimates atmospheric oxidation through reaction with hydroxyl radicals or ozone. The estimation methods are based on work by Atkinson and co-workers, and on a journal article that discusses the Atmospheric Oxidation Program (Meylan and Howard, 1993). For the calculation of the atmospheric half-life, a 12 hour (daytime) average concentration of 5E+6 OH-radicals/cm^3 is assumed. Reaction with ozone or other atmospheric degradation routes were not taken into account. In general, this atmospheric degradation route will not change the calculated atmospheric half-life significantly. It can however be an important factor specifically for unsaturated hydrocarbons, which are not halogenated around the carbon-carbon double bond. Thus, it is likely that the atmospheric half-life of this kind of substances will be overestimated.

The fraction of the substance sorbed to aerosol particles can be resistant to atmospheric degradation. Instead of correcting the half-life in air for sorption to aerosols (as implemented in the AeroWin programme which is also part of the US EPA EPISuite) the half-life in air is used directly in the OECD P_{ov}&LRTP Screening tool, as the multimedia model in this tool also corrects for sorption to aerosols.

All the QSAR estimation programmes mentioned above (KowWin, HenryWin, AOPWin, BioWin) are available in the EPISuite programme which is freely distributed by the US EPA [EPISuite 4.0, 2009]. A more detailed description of these and other models for the estimation of properties, and their potential relevance to the prediction of persistency and bioaccumulation, is presented in Appendix II of this report.

Centred, scaled and transformed P_{ov} – the P-score

The criterion for persistency in the POP frameworks or the vP-criterion in the REACH/PBT framework is a half-life of 180 days in soil or sediment, or 60 days in water. The calculated P_{ov} was centred around the criterion of 180 days, and scaled from 0 to 1, using a log-logistic equation:

$$P-score = e^{\frac{-\ln(2) \cdot 180}{P_{ov}}}$$

with P_{ov} as estimated by means of the OECD P_{ov}&LRTP Screening tool, in days.

Effectively, the scaling and centring is performed to be able to compare the P-score to other scores which are scaled over the same range (0-1). Centring on a P_{ov} half-life of 180 days reflects the choice in the regulatory setting for which this PB-score is developed. The log transformation is needed to diminish the influence of extremely persistent substances, with, e.g., P_{ov} half-life of tens of years, and gives a more equal distribution of all possible substances over the range of 0-1.

2.2.2 *Bioaccumulation*

The bioaccumulation factor (BAF) at the first trophic level in the food chain (birds and mammals) was chosen as the basis for the B-score. Although the regulatory frameworks often use bioconcentration factors (BCFs, for aqueous species) as threshold value in the POP or PBT assessment, this does not take into account possible trophic magnification through the food chain, and it ignores the potential for biomagnification specifically for air-breathing organisms. As the protection goal of PBT and POP assessments is focussed towards man and animals in more remote areas (birds and mammals like whales, or polar bears) the use of a bioaccumulation factor seems more relevant than the direct use of a bioconcentration factor in the calculation of a B-score. In order to not become overly conservative in the estimate of the bioaccumulation factor we have chosen the first trophic level (representative for animals like fish-eating birds, otters or seals). Animals like killer whales and polar bears (or humans) represent higher trophic levels, which would require higher trophic magnification factors. Moreover, by adding a trophic magnification factor for air-breathing organisms, substances that do not magnify in the pelagic food chain, but do substantially magnify in air-breathing organisms are assigned a higher score. These substances are characterized by a relatively low octanol-water partition coefficient and a high octanol-air partition coefficient (Kelly et al., 2007). A typical example of this group of substances is the POP lindane (γ-hexachlorocyclohexane).

Bioaccumulation factor – BAF

The bioaccumulation factor was estimated starting with the calculation of a bioconcentration factor based on the octanol-water partition coefficient of a substance. Subsequently this BCF was corrected for metabolism of the substance, and multiplied by a trophic magnification factor (TMF) which was estimated from the octanol-air partition coefficient (for air-breathing animals):

$$BAF_{(birds,mammals)} = TMF \cdot BCF_{metabolism\_corrected}$$

Calculation of the input parameters for BAF

Bioconcentration factor

The Gaussian function for the maximum BCF-value (median value) on the basis of the hydrophobicity (log K_{ow} in the following equation) for apolar organic chemicals in fish was retrieved from REACH Guidance R.11:

$$\log BCF_{\max} = \frac{34.43}{2.93 \cdot (2 \cdot \pi)^{0.5}} \cdot e^{-0.5 \cdot \left(\frac{\log K_{ow} - 6.52}{2.93} \right)^2}$$

The parameters in this equation are slightly different from those of the curve shown in Figure R11-4 of the REACH Guidance R.11, because in the calculations throughout this report the log K_{ow} was estimated by KowWin instead of ClogP. For the KowWin estimation see section 2.2.1.2

BCF corrected for metabolism

The maximum BCF-value represents a potential for bioconcentration and may provide a good estimate of the BCF-value for those substances that are effectively resistant to any metabolism in fish. Metabolism, however, may significantly reduce the bioaccumulation of a substance. In the most recent version of EPIWin, EPIWeb v4.0, an estimate for the half-life due to metabolism is calculated by the programme BCFBAF v3.00. The depuration rate constant due to metabolism (k_M) is directly calculated from this estimated half-life (k_M = ln(2) / $t_{1/2}$). To calculate the overall depuration rate constant, this depuration rate constant should be added to the depuration rate constant by passive diffusion ($k_{2,min}$).
The BCF is defined as the quotient of the uptake rate constant k_1 and the depuration rate constant k_2:

$$BCF = \frac{k_1}{k_2}$$

To be able to calculate a BCF adjusted for metabolism it must be realized that the estimated k_M from BCFBAF 3.00 is normalized to fish weighing 10 grams. According to Sijm et al. (1995) the uptake rate constant for substances with a log K_{ow} > 3 can be calculated from the weight of the fish using the following, which is also included in the REACH Guidance R.7c:

$$k_1 = 520 \cdot Weight^{-0.32}$$

Here, Weight is the normalized fish weight in grams. For a fish weighing 10 grams. Therefore this gives the (normalized) constant uptake rate constant k_1=248.9 L/kg/d.

For a maximum BCF-value (BCF_{max}), it can be assumed that the rate of metabolism (k_M) is zero. The minimum overall depuration rate constant can then be determined from the estimated uptake rate constant and the maximum BCF_{max}:

$$k_{2,\min} = \frac{k_1}{BCF_{\max}}$$

The overall depuration rate constant for substances that are metabolized can then be calculated as the sum of this minimum depuration rate constant and the rate constant for metabolism (as estimated with BCFBAF 3.00):

$$k_2 = k_{2,\min} + k_M$$

The metabolism-corrected BCF can then be calculated from the uptake rate constant and this elimination rate constant corrected for metabolism.

$$BCF = \frac{248.9}{\left(248.9 / BCF_{\max} + k_M\right)}$$

For substances with log K_{ow} < 3, the estimation of the uptake rate constant using the equation from Sijm et al. will lead to an *under*estimation of the influence of metabolism (k_M) on the BCF, which subsequently gives a conservative, worst-case estimate of the BCF of these non-lipophilic substances.

Trophic Magnification Factor

To include the concern for possible food chain transfer, especially in air-breathing organisms, such as mammals and birds, the biomagnification factor, expressed as trophic magnification factor, for these organisms was estimated from the octanol-air partition coefficient, K_{oa}. The following empirical relationship between the trophic magnification factor (TMF) and octanol-air partition coefficient, derived by Kelly et al. (2009), was used:

$$TMF = -0.753 \cdot (\log K_{oa})^2 + 13.0 \cdot \log K_{oa} - 46.2$$

The octanol-air partition coefficient is estimated by combining the HenryWin v3.20 model estimate for air-water partition coefficient, and the KowWin v1.67 model estimate for the octanol-water partition coefficient (see section 2.2.1.2). If the equation for TMF results in a value below 1, it is assumed that no trophic magnification occurs and the BCF is used as final BAF-value. In the estimate of the trophic magnification factor, no correction for metabolism was made. The estimated rate constant for metabolism is specific for fish and might not be directly applicable to other taxonomic groups, such as mammals. It is realized that mammals and birds probably have even higher metabolic capacities. However, since estimates of the (increased) metabolic rates for mammals are not available, and the estimate of the trophic magnification factor is not based on rate constants but uses an empirical correlation instead, making a correction for the metabolism in animals at the first trophic level is not possible.

Centred, scaled and transformed BAF – the B-score

The calculated BAF-value was centred around the criterion of 5000, used as the screening criterion for bioaccumulation in the POP frameworks and as the criterion for vB in the framework of REACH:

$$B - score = e^{\frac{-\ln(2)\cdot 5000}{BAF}}$$

Again, the log-logistic transformation function is used to achieve a more equal representation of all possible B-values over de range of 0-1, similar to the transformation used for P in section 2.2.1.3.

2.2.3 *Combining the P- and B-score into one PB-score*

Because the individual P- and B-scores have been centred, scaled and transformed, it is easy to combine the two scores into a single PB-score. The weight of the persistence criterion versus the bioaccumulation criterion for this study was chosen to be equal, i.e.

$$PB\text{-}score = P\text{-}score + B\text{-}score$$

The overall PB-score varies between 0 and 2. Substances with a PB-score of ≥1.5 will will have individual P or B-scores of at least 0.5 or higher, and therefore will be likely to comply with both criteria BCF ≥ 5000 and T½ ≥ 180 days. They may therefore be considered as potential POPs and vPvB substance candidates. Substances having a PB-score < 1.0 will not comply to the formal POP and vPvB criteria, as one of the individual P- or B-scores will be below 0.5. Substances with a PB-score between 1 and 1.5 might fulfil both criteria or not: e.g. P = 0.9 and B = 0.4 would (formally) not, but P = 0.7 and B = 0.6 would.

Although the BAF used in our methodology is not equal to BCF used for the (screening) criterion for bioaccumulation, and the P_{ov}-value is not equal to the half-life in one of the individual compartments which are defined as (screening) criteria for Persistence, it is thought that both the BAF and the P_{ov} better reflect the intrinsic potential of substances to have POP or PBT/vPvB concerns.
An estimate of the cut-off values for P- and B-score complying with the REACH PBT criteria (Table 2) is made, as if the (screening) criteria for REACH were defined using BAF and P_{ov}. The cut-off value for the P-score would formally not change compared to the POP criteria, as the worst case half-life for any compartment is equal for both the P and vP criteria, namely 180 days in marine sediment. Therefore, the P-score would also have to be $\geq$ 0.5 to be absolutely sure that the P criterion for considering a substance as P under REACH has been fulfilled (based on calculated half-lives). To reflect the less restrictive character for the P criteria when compared to the vP criteria, practically the less strict cut-off value of 120 days for half-life in fresh water sediment can be used. The P-score for a substance with a P_{ov} of 120 days would be 0.35.
The bioconcentration criterion changes from BCF>5000 for fulfilling vB criteria, to BCF>2000 for fulfilling the B criterion. In this exercise, BAFs are estimated instead of BCFs, but in order to have an idea of the cut-off value, BCF in the PBT criteria is replaced by BAF. For a substance with a BAF of 2000 a B-score of 0.18 is calculated.
In effect, this means that substances with an overall PB-score below 0.53 will not comply with the PBT criteria. The PB-score that needs to be reached to be absolutely certain that both criteria are fulfilled at the same time is 1.35. Substances with PB-scores between 0.53 and 1.35 might fulfil both criteria, but it could also be that they are extreme in one (P or B) and not reaching the threshold for the other property.

2.2.4 Applicability domain of the PB-score

Not all substances can be calculated using the methodology described in this study. The following groups of substances are expected to give no, or unreliable estimates of one or more of the properties used in the PB-score calculation:

- inorganic substances
- organo-metallic substances
- reactive substances (e.g. quickly hydrolyzing substances);
- salts;
- substances with very high molecular weight;
- surfactants;
- polymers.

Also, for substances of unknown or variable composition or biological origin (UVCBs), and for mixtures, it is not possible to make reliable estimates using the models applied in this study. However, if one or more individual components of a mixture or UVCBs are known, it is possible to make a PB-calculation for these individual components, and select the most representative PB-score (most probably the one giving the highest score). This approach is followed in Section 3.2.3 of the Results.

The OECD P_{ov}&LRTP Screening tool sets a limit on the acceptable range of the input parameters. This is indicated by a colour code. The range of acceptable input values is set (default) to:

-11	<	log K_{aw}	<	2
-1	<	log K_{ow}	<	10
1E-4	<	t1/2 soil(hours)	<	1E+10
1E-4	<	t1/2 water(hours)	<	1E+10
1E-4	<	t1/2 air(hours)	<	1E+10

Calculating P_{ov} for substances with properties outside this domain might give unreliable estimates, as the multimedia fate model is then forced to extrapolate very far.

2.3 Applying the PB-score to lists of commercial substances

2.3.1 Selection of lists

A database was created containing a broad range of substance types to be incorporated in the first screening on their POP criteria using the newly developed PB-score. It was decided to focus not only on the existing commercial (industrial) compounds that are present on the EINECS list, but to include pesticides (those registered either in the EU or in the US), biocides (EU) and active ingredients of pharmaceuticals (INNs in EU) as well. These substance groups were selected, since it is assumed that they may contain substances that fulfil the POP or PBT/vPvB criteria. An overview of the substance lists taken into account in the current study is given below.

The European database for New Substances (ELINCS) was not included, as for these substances no CAS number and molecular information is given, which is an initial condition for identifying physical-chemical characteristics of the substances using QSAR estimations as outlined in section 2.2. The OSPAR list, the so-called SIN list and the Canadian DSL list were not considered either, as it was assumed that they would not add any new entries to the already selected substance lists.

Throughout the report, the definition of substance as provided in REACH will be followed: 'Substance means a chemical element and its compounds in the natural state or obtained by any manufacturing process, including any additive necessary to preserve its stability and any impurity deriving from the process used, but excluding any solvent which may be separated without affecting the stability of the substance or changing its composition'. This is rather a legislative approach of the definition of substance instead of a substance definition. It should be realized that this approach has also been used in filling the ELINCS and EINECS databases, resulting in technical products, such as short-chained chlorinated paraffins, 'commercial' octa- and penta-bromodiphenyl ether, and natural products, such as coconut oil and fish oil, being classified as substances. Classification in the biocide, pesticide and pharmaceutical databases often focuses on the active ingredients.

Industrial chemical substances

For industrial chemical substances the EINECS (European Inventory of Existing Commercial chemical Substances) list was used. This list defines those chemical substances, which were deemed to be on the European Community market between 1 January 1971 and 18 September 1981. It was drawn up by the European Commission in application of Article 13 of Directive 67/548, as amended by Directive 79/831, and in accordance with the detailed provisions of Commission Decision 81/437. Substances on the EINECS list are called 'existing substances', whereas any chemical substance which has been marketed after 18 September, 1981 is called a 'new chemical'. Number of substances present on the list: 100.204.

Pesticides

Four databases were used to include as many pesticides as possible in our screening: the PAN Pesticide Database, the Alanwood database, the Ctgb list and the US-EPA pesticides database.

The PAN Pesticide Database brings together information on pesticides from many different sources, providing human toxicity, ecotoxicity and regulatory information for pesticide active ingredients and their transformation products, as well as adjuvants

and solvents used in pesticide products. The information is most complete for pesticides registered for use in the United States, reported by Pesticide Action Network North America (PANNA). Number of substances present on the list: 6.824 (of which 2.251 without a CAS number).
The Alanwood database provides details of the status of pesticide common ISO names, together with their systematic substance names, molecular formulae, structural formulae and CAS Registry Numbers. Number of substances present on the list: 1.860.
The Ctgb list is a database containing all authorized pesticides at the Board for the Authorization of Plant Protection Products and Biocides (Ctgb) in the Netherlands. Number of substances present on the list: 1.021.
The US-EPA pesticides database contains all registered pesticides at the Environmental Protection Agency in the United States. Number of substances present on the list: 606.

Biocides
EU regulation biocides: All active substances identified in Annex I as existing biocides in the European Union as reported by Commission Regulation (EC) No. 1451/2007 of 4 December 2007 were included in this screening. Number of substances present on the list: 900.

Pharmaceuticals
For pharmaceuticals the list of international non-proprietary names (INNs) which are free of duty in the European Union was used, provided by the World Health Organization, as reported by Commission Regulation (EC) No. 1031/2008 of 19 September 2008 (Annex 3). Number of substances present on the list: 7.535 (of which 44 without a CAS number).

2.3.2 *Chemical structure information*

All lists taken together resulted in a total of 119.557 potential substances. The overlap of substances on the lists reduced this number to 107.337 unique CAS numbers (the overlap between the various lists is therefore 12.220 substances). For 69.152 out of these 107.337 CAS numbers, a single representative chemical structure could be (automatically) assigned. As already indicated, the EINECS list contains a large number of technical products, consisting of mixtures of chemical substances, as well as natural products, which have a CAS number assigned, but for which it is not possible to link their CAS numbers to a single representative chemical structure. Also, for several CAS numbers structure information could not be generated in an automated way, although the CAS-RN belongs to a well defined single chemical structure. Only for CAS-RN numbers for which a chemical structure was available in a (digital) table, the different P- and B-properties were estimated. This does not mean that for the other substances it is not possible to make estimations, but this requires entering structure information by hand. This has been performed when evaluating the performance of the score, for several structures and isomers that were not present on the combined list of chemicals

Structure information was derived from four data sources:
- EINECS QSAR optimized structures as provided by the ECB; 59.922 (single, defined) structures for 101.176 substances on the EINECS list,
- SMILESCAS.db from Syracuse Inc. (makers of EPIWIN suite for the US-EPA, ~112.000 CAS registry numbers with structure information),
- NCI database (>250.000 chemical structures, of which 126.205 have a CAS registry number assigned to them),

- In-house list of CAS-SMILES containing about ~65.000 CAS registry numbers with structure information (SMILES), the sources of this data are mixed/unknown.

The reliability of the chemical structure information sources was considered to be:

EINECS > SMILECAS > NCI > In-house list

The structure of the substance was retrieved from the source that was assigned the highest reliability, the EINECS database. If a structure could not be assigned to a CAS-RN using this first source, the next most reliable source was used. Since the source of the data on the 'in–house' list was not known, it was used as the 'last resort', in case the other three sources could not provide a structure. No specific quality check on the chemical structure information has been performed, not for single substances, nor when a structure could be assigned using more than one of the above four sources.

Finally, from the 69.152 single chemical structures, a PB-score could be calculated for 64.721. The remaining structures were not accepted by one or more of the applied QSAR methods, or the (calculated) properties were too extreme for the OECD LRTP model to allow calculation of a reliable overall persistence. The number of CAS numbers and assigned structures is presented in Table 3 for the individual lists used in this exercise as well as for the combined list of substances.

2.4 Evaluation of performance of the new PB-score

Evaluation of the performance of the new PB-score (and the individual P- and B-score) was performed by comparing the P- and B-scores of the UNECE POP substances and the nominations with the cut-off values complying with the formal screening criteria ($P \geq 0.5$ and $B \geq 0.5$). A further evaluation is performed by comparing the rank of the POP substances and the nominations according to their PB-scores with the rank of all other substances on the selected lists.

Information on the decision of the EU PBT working group on 127 potential PBT substances which have been evaluated within the European New and Existing Substances Frameworks, i.e. before June 2008, was used to evaluate the current methodology as well. The individual P- and B-scores were used to conclude whether a substance should be classified as PBT or vPvB, or if it should be removed from the potential PBT list based on (estimated) non-persistency or non-bioaccumulation potential.

Table 3. Numbers of substances on the lists taken into account in this study, and number of substances with a single chemical structure assigned to this CAS number. The REACH definition of substance is applied

Substance group	Description	Number of substances	Nr. single structures assigned	Reference
Existing commercial chemicals	EINECS list	101.176	61.270	O.J. C 146A, 15.6.1990 Corrections: O.J. C 54/13 01.03.2002, 2002/C54/08
Pesticides	PAN database	6.588	5.923	http://www.pesticideinfo.org/
Pesticides	Alanwood db	1.840	1.317	http://www.alanwood.net/pesticides/sitemap.html
Pesticides	Ctgb database	998	770	http://www.ctb.agro.nl/portal/page?_pageid=33,%2047131&_dad=portal&_schema=PORTAL
Pesticides	US-EPA database	602	405	EPA/OPP Conventional Pesticide Cases: Registration Review Schedule dd. 12-15-08
Biocides	EU regulation	880	727	COMMISSION REGULATION (EC) No. 1451/2007. 4 December 2007. ANNEX 1
INNs: Active ingredients pharmaceuticals	EU regulation	7.473	4.714	COMMISSION REGULATION (EC) No. 1031/2008. 19 September 2008 ANNEX 3: l_29120081031en00010894.pdf
	All	119.557	75.126	Total number of entries in all lists (section 2.3.2)
	All	107.337	69.152	Substances with a unique CAS nr., represented by a single representative structure (section 2.3.2)
	All		**64.721**	**Substances for which P- and B-score could be calculated (section 3.1)**

3 Results

3.1 PB-scores for substances on lists of commercial substances

The results of the calculations were tabulated in a Microsoft Excel worksheet, which can be used as a quick 'look-up' tool to determine the P-, B-, and combined PB-score of a given substance by entering its CAS-RN. The output also contains all the estimated properties and their interpreted values such as half-lives, overall persistency P_{ov}, BCF_{max}, TMF and BAF. This information is instructive when interpreting the calculated P-, B- and combined PB-scores. A CAS number is needed to look up substances. This information also forms the basis of a database enabling searching and filtering on chemical structure or chemical similarity. In this database, it is also possible to search for chemical structures without having to assign a CAS number in advance, and it enables searching for chemically similar substances for which the P-, B- and PB-scores have been pre-calculated.

The total number of substances fulfilling the POP criteria, the vPvB criteria and the PBT criteria based on their calculated properties, are provided in Table 4. Estimates of the cut-off criteria for the calculated P- and B-scores for fulfilling the respective POPs, vPvB and PBT are given in chapter 2.2.3.

Table 4 The minimum number of substances among 64.721 substances that fulfil the POP, vPvB and PBT criteria based on their calculated properties.

Criterion	Number of substances
POP and vPvB criteria	
P ≥ 0.5	16.646
B ≥ 0.5	4.748
P ≥ 0.5 and B ≥ 0.5	1.986
PB(T) criteria	
P ≥ 0.35	23.460
B ≥ 0.18	8.371
P ≥ 0.35 and B ≥ 0.18	4.541

3.1.1 The highest PB-scores

Overall, 1.986 (out of the 64.721 for which a PB-score could be calculated) substances have both their P- and B-score above 0.5, indicating that these substances meet the POP and vPvB criteria based on their calculated properties.

The 250 highest scoring substances are listed in Appendix 4 along with their estimated properties. The 30 top-ranking substances according to their combined PB-score are presented in Table 5. Both in Appendix 4 and in Table 5, the UNEP/UNECE POP-substances, POP-nominees and PBT-substances (see sections 3.2 and 3.3) are indicated in bold.

Table 5 PB-scores for the top-31 substances from lists of existing (commercial) substances

Rank	CAS	Name	P-score	B-score	PB-score
1	93819-97-7	perfluorinated octanoic acid (PFOA) derivative?	1.00	0.99	1.99
2	**2385-85-5**	**Mirex**	**1.00**	**0.98**	**1.98***
3	39765-80-5	Nonachlor	0.99	0.99	1.98
4	10386-84-2	4,4'-Bromo-octafluorobiphenyl	1.00	0.98	1.98
5	**5566-34-7**	**Gamma-Chlordane**	**0.99**	**0.98**	**1.98**
6	18291-67-3	Hexachloro-6-(methyldichlorosilyl)norbornene	0.99	0.98	1.97
7	2550-75-6	Chlorbicyclen	0.99	0.99	1.97
8-10	**57-74-9**	**Chlordane (technical, cis- and trans-)**	**0.99**	**0.97**	**1.97**
11-16	-	perfluorinated octanoic acid (PFOA) derivatives	0.98	0.98	1.97
17	**8001-35-2**	**Toxaphene**	**0.99**	**0.97**	**1.96**
18	78974-42-2	perfluorinated octanoic acid (PFOA) derivative	1.00	0.96	1.96
19	18106-12-2	diethoxy-(1,2,3,4,7,7-hexachloro-5-bicyclo[2.2.1]hept-2-enyl)-methylsilane	0.98	0.98	1.96
20-24	67584-62-7	perfluorinated octanoic acid (PFOA) derivatives	0.98	0.98	1.96
25	18300-04-4	dibromo-Chlordene	0.98	0.97	1.96
26	68412-68-0	perfluoroalkyl(C6-C10)phosphinic acid	0.99	0.96	1.96
27	13252-14-7	perfluorinated octanoic acid (PFOA) derivative	0.98	0.98	1.96
28-29	**309-00-2**	**Aldrin (2 different CAS nrs.)**	**0.97**	**0.98**	**1.96**
30	68555-67-9	perfluorinated octanoic acid (PFOA) derivative	0.99	0.96	1.95
31	68631-02-7	tetrachloro-DDT	0.97	0.98	1.95

* UNEP and UNECE POP substances, indicated in **bold**

The highest PB-score of all substances is calculated for an EINECS entry, which is available on the market, but the function or uses of which can not easily be determined. It is a substance with a perfluoro-alkyl chain, which explains the high persistence of the substance. Its structure and IUPAC name are presented in Figure 2.

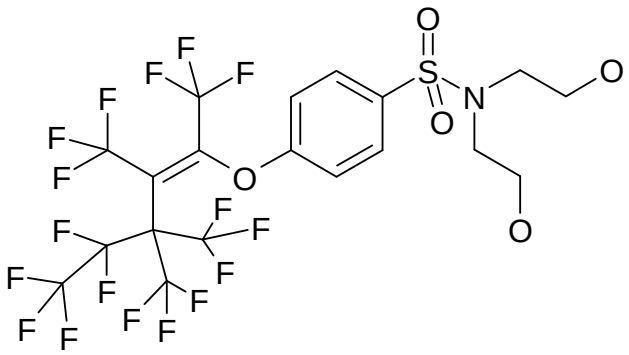
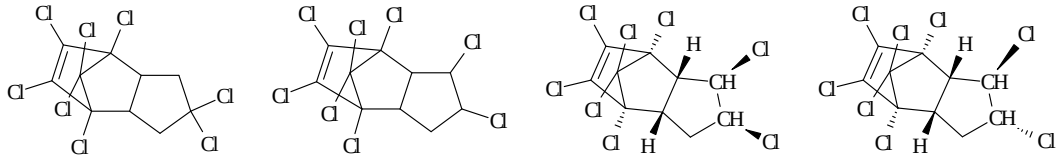


Figure 2. Substance with rank 1 on the PB-score: EINECS nr. 298-581-0 N,N-Bis(2-hydroxyethyl)-4-((4,4,5,5,5-pentafluoro-3-(pentafluoroethyl)-1,2,3-tris(trifluoromethyl) pent-1-enyl)oxy)benzenesulphonamide

The second highest scoring substance in the list is *Mirex*, a well known Persistent Organic Pollutant (POP) which is present on the official UNECE/UNEP list of POP substances. The third substance, *Nonachlor,* is very similar to *Heptachlor*, which is officially recognized as a POP substance. Heptachlor itself ranks as number 36 of the 64.721 substances (see Appendix 4). In the Top-30 three more POPs are found: *Chlordane* with four separate CAS entries, *Toxaphene* on rank 17, and *Aldrin* which was present in this exercise under two different CAS numbers. The complete lists of confirmed POPs and POP nominations with their PB-scores and ranks are presented in section 3.2.

It is interesting to note that a substance like Chlordane is represented by four different CAS numbers on the lists used in this study. The four different forms of chlordane are presented in Figure 3 with their respective CAS numbers. Three out of the four Chlordane CAS entries – the technical mixture, cis-chlordane (or α-chlordane) and trans-chlordane (or β-chlordane) have completely identical scores calculated. Their chemical structure information is not completely similar, as the steric conformation (cis- and trans-) is distinguished in this exercise. The QSAR models that are used for the calculation of the properties, however, do not distinguish between sterical isomers, leading to exactly similar P- and B-scores for the cis- and trans-form and the racemic mixture. The reason that γ-Chlordane gets a different, slightly higher PB-score is due to the fact that this is a different chemical congener, not a sterical isomer.

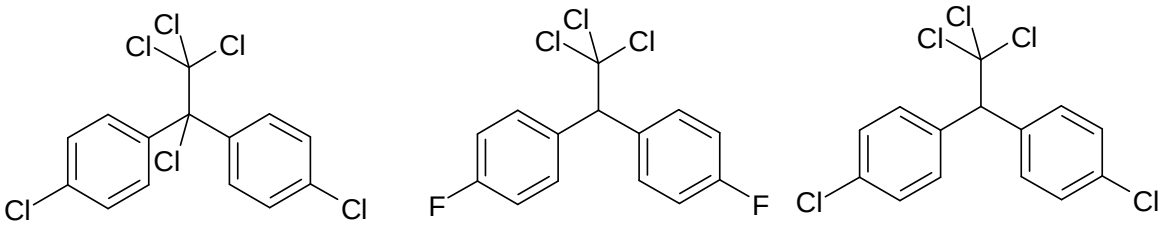


Name:	γ–chlordane	chlordane (techn.)	α–chlordane	β–chlordane
CAS nr.:	5566-34-7	57-74-9	103-71-9	103-74-2
PB-score:	1.98	1.97	1.97	1.97
Rank:	5	8	9	10

Figure 3. Four structures of Chlordane with different CAS registration numbers

The last substance in Table 5, tetrachloro-DDT, is very similar in chemical structure to the well known POP substance DDT. Its structure is presented in Figure 4 together with DDT and another DDT-like substance (DFDT). DDT itself ranks as nr. 82 (of all 64.721 structures evaluated) with a PB-score of 1.92 (see Appendix 4). The PB-score quantitatively distinguishes DDT from its close structural analogue, which has only one choro-atom extra. This extra chloro-atom apparently increases the (calculated) persistence and bioaccumulative properties of the substance, yielding an increase in PB-score from 1.92 to 1.95. It is, however, questionable whether a quantitative difference in persistence and/or bioaccumulation behaviour between these two substances could be observed in the environment.

The most 'borderline' substance according to its PB-score would be p-(p-nitrophenoxy)anisole, CAS 6337-24-2, with both a P-score of 0.50 (overall persistence P_{ov} = 181 days) and a B-score of 0.50 (BAF = 5028).



Name:	tetrachloro-DDT	DFDT	DDT (POP)
CAS nr.:	68631-02-7	475-26-3	50-29-3
PB-score:	1.95	1.94	1.92
Rank:	31	51	82

Figure 4. DDT and two close structural analogues, tetrachloro-DDT, and DFDT with their ranking within the list of ~65.000 evaluated structures, together with the absolute PB-scores.

3.1.2 Most persistent substances – highest P-scores

When the 64.721 substances are ordered according to their P-score, it turns out that there are 498 substances with a P-score of 1.00, and almost all are perfluorinated or highly fluorinated substances. One of the few non-fluorinated substances in this top-500 is Mirex, which ranks as number 174 based on the P-score alone. Chlordane is the second POP-substance at place 634, with a P-score of 0.99.

3.1.3 Most bioaccumulative substances – highest B-scores

The highest score in the list of 64.721 existing substances based on B-score would be 1,4-dibutoxy-2,5-dichlorobenzene (CAS RN 68052-14-2). This substance (shown in Figure 5) has a B-score of 0.9905. Its P-score is 0.32. Its overall persistence (P_{ov}) was calculated to be 111 days. Based on its combined PB-score of 1.31 it is ranked as number 1.760.

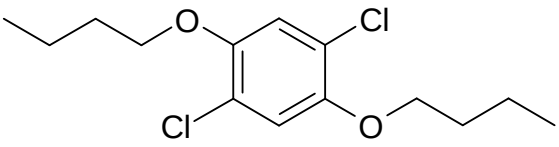


Figure 5. 1,4-dibutoxy-2,5-dichlorobenzene, CAS nr. 68052-14-2, EINECS 268-307-4 PB-score 1.31, B-score 0.99, P-score 0.32.

The Top-50 based on B-scores alone resembles the list of top PB-scoring substances (presented in Table 5) rather than the Top-50 based on P-scores. It is interspersed with substances that have relatively low P-scores, such as the substance in Figure 5. Also, the same UNEP/UNECE POP substances (Mirex, Chlordane, Toxaphene, Aldrin) rank high within the top-50, on the basis of their B-scores alone.

A commercially interesting substance which scores very high on calculated bioaccumulation potential (B-score 0.98, ranked as nr. 85 based on B-score), but which is hardly persistent, is retinoic acid (vitamin A).

3.1.4 *Highest PB-scores for pharmaceuticals (INN list)*

Substances which have been selected for our screening exercise have been registered once as a commercial substance (e.g. on EINECS, in a pesticide registration system or as a biocide), making it necessary to check the present status of the substance and to investigate if they are still being marketed and if so, in what volume. On the other hand, the pharmaceutical compounds list (INN list) only contains substances that are actually currently being marketed, although their volume on the market can vary greatly. Pharmaceuticals scoring high on the PB-score are therefore immediately more interesting candidates for further investigation. However, pharmaceuticals are not expected to have very extreme log K_{ow} properties (as e.g. reflected by Lipinsky's 'Rule of 5', Lipinsky et al. 1997), and therefore, it is not likely that they are present in large numbers in the first couple of hundred highest scoring substances, as indicated by the ten INN list substances in Table 6. Among the 250 highest scoring substances based on their PB-score (Appendix 4) only six INN list entries were found.

Table 6 Highest 10 PB-scores for pharmaceuticals as registered on the INN list

Name	CAS nr	PB-score	P-score	B-score	Pharmaceutical Use	Rank
Dieldrin	60-75-1	1.94	0.97	0.97	Insecticide	48
Bromocyclene	1715-40-8	1.93	0.97	0.97	Veterinary, insecticide	53
DDT	50-29-3	1.92	0.94	0.98	Insecticide	82
Fletazepam	34482-99-0	1.88	0.95	0.93	Insomnia treatment	132
Perfluamine	338-83-0	1.82	1.00	0.82	Respiratory distress, ophthalmic use	200
Mitotane	53-19-0	1.82	0.85	0.97	Antineoplastic	210
Perflunafene	306-94-5	1.79	1.00	0.79	Respiratory distress, ophthalmic use	263
Penmestrol	67-81-2	1.77	0.83	0.95	Steroid	291
Perflexane	355-42-0	1.77	1.00	0.77	Contrast medium	293
Enoxolone	471-53-4	1.74	0.91	0.83	Anti-viral, -bacterial, anti-allergic	327

The highest ranking substance present on the INN list is *Dieldrin*, and the third substance is *DDT*. Both used to have veterinary uses (insecticide) before they were banned. The second highest ranking substance from the INN list is *Bromocyclene*, also a veterinary medicine, which is used as a non-specific insecticide, e.g. against fleas.

Fletazepam is the first human pharmaceutical of the highest PB-scores on the INN list. It is a benzodiazepine derivative, has sedative and anxiolytic effects ('tranquilizer'), and has strong muscle relaxant properties.

Mitotane (o,p'-DDD, a DDT metabolite) is an antineoplastic that directly suppresses the adrenal cortex. It may also modify peripheral steroid metabolism. It is given in the treatment of advanced adrenocortical tumours.

Perfluamine and *Perflunafene* are highly fluorinated compounds, which can absorb, transport, and release oxygen and carbon dioxide. Intra-ocular injections of perflunafene, alone or combined with other perfluorocarbons, are used to provide a temporary tamponade in ophthalmic procedures such as retinal re-attachment.

Perflunafene and perfluamine have been used together for their oxygen-carrying properties in blood substitute preparations and to prevent myocardial ischaemia during percutaneous transluminal coronary angioplasty.

Penmestrol, or methyltestosterone, is a steroid structure, having anabolic and androgenic properties. Other steroid structures are present in the top of the PB-scoring substances, e.g. Erythrodiol, a phytosterol, rank 246, CAS nr. 545-48-2. Steroid structures which are thought to be highly persistent and bioaccumulative should give rise to serious concern, as the hormonal, endocrine disrupting properties of these structures give a very high potential of toxic effects at very low exposure concentrations. These long-term effects at very low concentrations were the very reason to start doing POP, PBT and vPvB assessments, as it is thought that the (environmental) risk of such substances will not necessarily be recognized through regular, quantitative, risk assessment of substances. Enoxolone (see below) also has a steroid ring structure.

Perflexane, or perfluorohexane, is a perfluorocarbon gas that has been used as an ultrasound contrast medium for echocardiography. Dry microspheres containing the gas are reconstituted immediately before use, leading to the formation of microbubbles of perflexane that provide echo-enhancement; lipids are included in the microspheres to stabilize the bubbles when they form.

Enoxolone, which has a steroid ring structure, is used locally in preparations for the treatment of non-infective inflammatory disorders of the skin, mouth, throat, and rectum. Enoxolone potassium (potassium glycyrrhetinate) has been used similarly. Derivatives of enoxolone, including its aluminium salt have been used in the treatment of benign peptic ulcer disease and other gastrointestinal disorders.

From the 1.986 substances having both their P-score and their B-score above 0.5, there were 92 substances from the INN list of pharmaceuticals. These 92 pharmaceutical substances are the minimum set of INN list entries which formally meet the POP and vPvB criteria according to their calculated properties.

3.2 PB-scores for UNEP/UNECE POPs

3.2.1 Existing POPs

The score and the ranking of the agreed UNEP and UNECE LRTAP POPs, with their rank in the list of 64.721 evaluated substances, is presented in Table 7. Out of the 17 official POP substances which are not mixtures, 11 are ranked among the top-250 of the substances evaluated (Table 7, Appendix 4). Out of those 17, 16 comply with the formal screening criteria for UNEP/UNECE POPs according to their calculated P- and B-scores; these 16 have both P- and B-scores above 0.5 (Overall persistence half-life is estimated to be > 180 days and Bioaccumulation factor is estimated to be > 5000).

Only *Hexabromobiphenyl* would not pass the formal screening criteria for POPs based on its calculated properties. Based on the P-score of 0.96, hexabromobiphenyl is considered to be very persistent. However, according to the calculations, hexabromobiphenyl is not likely to strongly bioaccumulate. This substance only scores 0.10 for the B-score, which is due to the high estimated log K_{ow}-value of 9.1. Thus, it would be expected to result in a reduced uptake and a maximum BCF-value of around 1500. The ClogP estimation programme calculates a much lower log K_{ow} of 7.81 for this substance, leading to a much higher B-score of 0.80, resulting in a PB-score of 1.76 instead of 1.06. This example stresses the fact that the outcome of the score is very dependent on the reliability of the QSAR estimates.

Table 7 UNEP and UNECE LRTAP POPs Annexes I, II and III of the Stockholm convention, with their respective P-, B- and PB-scores and their rank among the 64.721 precalculated substances.

POP	CAS RN	Annex	PB-score	P-score	B-score	Rank
Mirex	2385-85-5	I	1.98	1.00	0.98	2
Chlordane	57-74-9	I	1.98	0.99	0.98	5
Toxaphene	8001-35-2	I	1.96	0.99	0.97	17
Aldrin	309-00-2	I	1.96	0.97	0.98	28
Heptachlor	76-44-8	I	1.95	0.97	0.98	36
Endrin	72-20-8	I	1.94	0.97	0.97	47
Dieldrin	60-57-1	I	1.94	0.97	0.97	48
DDT	50-29-3	I + II	1.92	0.94	0.98	82
Perfluorooctanesulfonate (PFOS)	1763-23-1	II	1.89	0.94	0.95	116
Chlordecone	143-50-0	I	1.85	1.00	0.85	163
Hexachlorobenzene (HCB)	118-74-1	I + III	1.85	0.92	0.93	170
Pentachlorobenzene (PeCB)	608-93-5	I + III	1.72	0.84	0.88	375
Hexachlorocyclohexane (techn.)	608-73-1	II	1.67	0.87	0.80	488
α-HCH	319-84-6	I	1.67	0.87	0.80	485
β-HCH	319-85-7	I	1.67	0.87	0.80	486
γ-HCH, Lindane	58-89-9	I	1.67	0.87	0.80	484
Hexabromobiphenyl	36355-01-8	I	1.06	0.96	*0.10*[a]	3587
Pentabromodiphenyl ether (PeBDE, commercial)	Mixture[b]	I	n.a.			n.a.
Octabromodiphenyl ether (OctaBDE, commercial	Mixture[b]	I	n.a.			n.a.
Polychlorinated biphenyls (PCBs)	Mixture[b]	I + II	n.a.			n.a.
Polyaromatic hydrocarbons (PAHs)	Mixture[b]	III	n.a.			n.a.
Dioxins/Furans (PCDDs/PCDFs)	Mixture[b]	III	n.a.			n.a.

[a] P- or B-score in *italics* indicates that the score does not comply with the POP status of a substance, see table 4

[b] Individual components to be evaluated manually. See section 3.2.3, and Table 9 for PB-scores of the respective individual components of these mixtures)

n.a. A single PB-score and a rank are not available for mixtures

PFOS is calculated to have a PB-score of 1.89, and it ranks as number 116 in the list of evaluated substances. It is ranked among the top POP and PBT candidates, but it should be noted that the perfluorooctanoic acid derivatives consistently score very high with this methodology. In the Top-30 (table 5, section 3.1) there are several PFOA derivatives present. Some are very close structural anologues and true PFOA derivatives, others have varying perfluoro-alkyl chain length and cannot be seen as real PFOA derivatives in a chemical sense. E.g. the substance ranking number 18 in Table 5 is 3,3,4,4,5,5,6,6,7,7,8,8,9,10,10,10-Hexadecafluoro-9-(trifluoromethyl) decyl dihydrogen phosphate, with an alkyl chain length of 10 (instead of 8), and it is a phosphate, not a sulphate. All these substances are considered to be of the same type (PFOA derivatives). Nevertheless, the high ranking of the perfluoro compounds is in a sense unexpected, because the bioaccumulation potential of these substances is not thought to be driven by its partitioning into lipids, but instead mainly by binding to proteins. The B-score is based on the log K_{ow} as a surrogate for lipid partitioning, and the estimated log K_{ow}-values for the perfluoro compounds are in a range to have a high lipid partitioning bioaccumulation potential. Combined with the correctly predicted high environmental half-life and high half-life for metabolism in fish, this leads to a high final PB-score. However, a closer look at the log K_{ow}-values estimated by KowWin leads to the conclusion that the calculated values are probably higher than realistic for these surface active perfluorinated compounds. Indeed ClogP

predicts much lower values than KowWin, e.g. 2.27 for PFOS instead of 6.28, and 3.62 for PFOA instead of 6.30. This difference between these two estimation methods is due to the the fact that KowWin calculates the log K_{ow} for the neutral species, whereas ClogP assumes complete ionization (which is probably more accurate in this case). Experimental log K_{ow}-values for these substances are hard to determine due to their surface activity. It must be concluded that the QSAR estimates for perfluorinated substances from KowWin lead to a high PB-score by accident, although their persistence and lack of metabolism are correctly estimated.

Hexachlorocyclohexane (HCH, Lindane), which does not officially meet the formal bioaccumulation screening criteria, does score very high in the ranking based on the PB-score. The log K_{ow} of HCH is calculated (and measured) to be (slightly) below the screening value of 4.5, and also the BCF-value as calculated e.g. by the BCFWin estimation programme [EPA] and as used in the EPA PBT profiler, would give a BCF-value well below the screening value of 5000. The fact that HCH does rank very high in the PB-score is due to the fact that biomagnification for air-breathing organisms is taken into account in the calculation of the BAF, and subsequently is expressed in the B-score as well.

PCBs as listed within the two POP conventions are (technical, commercial) mixtures of individual polychlorinated biphenyl congeners. Mixtures can be represented by a single CAS number, however, it is not possible to assign a single chemical structure to this CAS-RN. The individual congeners each will also each have their own CAS number assigned to them, but these are not present in our list of substances to be evaluated, as the individual congeners have not always been registered as commercially interesting substance(s) e.g on the EINECS list. Mixtures such as *PAHs* (polyaromatic hydrocarbons), *PCDDs* and *PCDFs* (polychlorinated dioxins and furans) and *commercial Penta-* and *Octa-bromobiphenyl ether* mixtures can be evaluated manually by evaluating the individual congeners or constituents. See the results of calculations for POP mixtures in section 3.2.3, Table 9, and in chapter 4, Discussion.

3.2.2 POP nominations

In recent years a number of substances have been proposed as UNECE LRTAP and UNEP POPs. Their P- and B-scores and ranks among the list of 64.721 substances evaluated in this study are presented in Table 8, on the next page.

Hexabromocyclododecane (HBCDD) initially received a P-score of 0.92 and a B-score of 0.30, placing it relatively low in the ranking at place 2343. The B-score of 0.3 corresponds to a calculated BAF of 2850, which would not meet the formal POP criterion of 5000. This BAF is relatively low because a relatively mild trophic magnification is expected (TMF of 1.3) and a metabolic half-life of 7 days is estimated for this substance. It should be noted that the representative structure assigned to the CAS number for HBCDD was 1,1’,2,2’,3,3’-hexabromocyclododecane, which is probably not the best representation of the actual congeners found in technical HBCDD. Another HBCDD structure is present on the EINECS list under CAS number 3194-55-6. The structure assigned to this CAS number in this exercise is 1,2,3,4,7,8-hexabromocyclododecane. The P-score for this congener was 0.72, compared to 0.92 for the former congener, but the B-score increases to 0.84 instead of 0.30, leading to an overall PB-score of 1.55, which is markedly higher. CAS numbers 25637-99-4 and 3194-55-6 refer to 1,3,5,7,9,11- and 1,2,5,6,9,10-hexabromocyclododecane, respectively, according to the PubChem registry. For these specific congeners of HBCDD the B-scores are relatively high as well, with 0.72 and 0.94, respectively. The last structure is thought to be most representative of HBCDD (with the stereoisomers α, β, γ and δ, which will all receive the same PB-score).

Table 8 UNEP and UNECE LRTAP POP nominations

POP Nomination	CAS RN	Year	PB-score	P-score	B-score	Rank
Hexabromocyclododecane (HBCDD)		2005				
1,1',2,2',3,3'-HBCDD	(25637-99-4)		1.22	0.92	*0.30*[a]	2343
1,2,3,4,7,8-HBCDD	(3194-55-6)		1.55	0.72	0.84	761
1,3,5,7,9,11-HBCDD[b]	25637-99-4		1.46	0.74	0.72	~1078
1,2,5,6,9,10-HBCDD[b]	3194-55-6		1.68	0.74	0.94	~470
Short chain chlorinated paraffins (SCCPs)	85535-84-8	2005	[c]			
Polychlorinated naphthalenes (PCNs)	Various	2005	[c]			
Dicofol	115-32-2	2008	1.89	0.95	0.94	109
Pentachlorophenol (PCP)	87-86-5	2008	1.27	0.85	0.42	2009
Pentachloroanisole (PCP-metabolite)[b]	1825-21-4		1.84	0.88	0.97	~172
Endosulfan	115-29-7	2008	1.34	0.86	0.47	1577
Hexachlorobutadiene	87-68-3	2008	1.32	0.85	0.46	1751
Trifluralin	1582-09-8	2008	1.05	0.90	*0.15*[a]	3637

[a] P- or B-scores indicated in *italics* indicate that these scores do not comply with the assumed POP status of the nominated substance (see table 4).

[b] Two HBCDD congeners and Pentachloroanisole were not part of the list of 119.521 commercially registered substances and have been calculated manually. Their ranks are therefore an approximation.

[c] Individual components of these mixtures to be evaluated manually (see section 3.2.3 and Table 9)

Experimental data indeed indicate a very high bioaccumulation potential throughout the whole food chain for HBCDD, with BCF-values in fish already amply exceeding 5000 and significant biomagnification. It is clear in this case that the structure assigned to the CAS number for HBCDD might not be the most representative when trying to identify the worst-case P and B properties. When using a CAS number as a look-up for the PB-score, it should always be checked if the structure assigned to the CAS number represents the relevant isomer/congener/component in the mixture. A much better, but also much more elaborate way to evaluate mixtures is to calculate a separate PB-score for each individual isomer/congener/component in each substance. This approach is presented in the next section (3.2.3) for the POP-mixtures.

The B-scores for *endosulfan* (0.47)*, hexachlorobutadiene* (0.46) and *pentachlorophenol* (0.42) are relatively close to the cut-off value of 0.5 which represents a BAF of 5000, the formal screening criterion for POPs. Given the margin of error in the calculation of the BAF (and underlying log K_{ow}, log K_{aw} and BCF), these substances may still bioaccumulatie sufficiently to meet the POP criteria.. For pentachlorophenol it should be noted that this substance is mainly of concern because of the POP properties of its metabolite, pentachloroanisole, and impurities like polychlorinated dioxins, dibenzofurans and hexachlorobenzene. Indeed, the metabolic half-life estimated for pentachlorophenol is relatively rapid, 2.2 days. This adjusts the calculated BCF_{max} from 15.000 to a metabolism corrected BCF of 751. Moreover, at neutral pH pentachlorophenol will be ionized, which further reduces its bioaccumulation potential. *Pentachloroanisole* (CAS 1825-21-4) was not present in the list of 119.521 substances, as it is not a commercially registered product (see 2.3.2). Its PB-score has been calculated separately. The PB-score of pentachloroanisole is calculated to be 1.84, which would rank around place 171 in the list of existing substances. Specifically the difference in B-score for pentachlorophenol (B-score 0.42) and pentachloroanisole (B-score 0.98) is very significant, and indicates the importance and influence of (persistent) metabolites.

Trifluralin has a relatively low B-score of 0.15. This is mainly due to the estimation that trifluralin can be metabolized rapidly in (aquatic) organisms. The metabolic half-life for trifluralin is estimated to be 0.6 days. This estimated rapid metabolism gives a significant correction of the BCF_{max}, which, based on a log K_{ow}-value of 5.34, is calculated to be as high as 20.090. The metabolism corrected BCF using a metabolic half-life of 0.6 days becomes 200, showing that the influence of the estimated metabolic rate can be very drastic. Probably N-dealkylation of the amino-group in trifluralin is relatively easy and rapid, but might give rise to stable metabolites of trifluralin, which could still have bioaccumulative properties. However, N-dealkylation followed by rapid excretion of trifluralin has been shown experimentally in rats [Erkog, 1985].

3.2.3 POP-mixtures

For estimating a PB-score using the method described in chapter 2 it is necessary to have one specific chemical structure assigned to the substance of interest. Commercial mixtures are often represented with a single CAS number for the whole mixture. Since this CAS number can not be described with one single chemical structure, it is often not present in the chemical structure lists used in this exercise. Some CAS numbers for mixtures were automatically assigned a 'representative' structure in this study. This automatically assigned structure is not always the structure which is best representing the potential P- and B-properties of a mixture. This is for instance the case with SCCP (CAS RN 85535-84-8). For most mixtures single representative structures have to be assigned manually to the constituents of the mixture and their individual CAS numbers. Knowledge about the relative percentages of the constituents in the mixture is indispensable for identifying if the constituents are present in relevant quantities.

For this study, the component of a mixture that is present in volume >1%, and which has the highest scoring P- and B-properties as expressed by the PB-score, is thought to represent the mixture best considering its POP/vPvB characteristics. The 1% is well above the amount which could be considered to be an unintentional trace amount (see UNEP/POP/POPRC6/INF/19). This approach is especially useful when the percentage of each component in the mixture is known and if the components fulfilling the criteria add up to a relevant percentage.

To see the trends for P and B within a mixture, a number of different components will have to be calculated manually, and subsequently it should be determined which component is likely to have the highest PB-score. Most of the mixtures which are POPs or nominated as POPs have mixture components with varying degrees of halogenation. In general the highest halogenated component will also be the most persistent, but with regard to bioaccumulation, there is an optimum in log K_{ow} and log K_{oa} leading to the highest B-score. The most halogenated component in a mixture could have such a high (calculated) log K_{ow}-value that the B-score will be (very) low. The best approach is to calculate PB-scores for each individual component present in a mixture, and select the highest PB-score of an individual component to represent the mixture. For several mixtures this exercise has been performed. All POPs or POP nominations which are mixtures are listed in Table 9. Most mixtures from the list of confirmed and nominated POPs have been worked out in detail. Others could still be evaluated in further detail, as only one or a few high scoring components of the mixture are given. The scores illustrate the compliance of the highest PB-score of a mixture with the POP or POP nomination status. The results of the calculations for POP mixtures are discussed following Table 9.

Table 9 UNECE POPs and nominations which qualify as (technical) mixtures

Mixtures and their component(s)	**CAS RN**	**PB-score**	**P-score**	**B-score**	**Rank**
DDT in Dicofol		**1.89-1.92**			**82**
Dicofol	115-32-2	1.89	0.95	0.94	109
DDT	50-29-3	1.92	0.94	0.98	82
Polychlorinated naphthalenes (PCNs)		**0.67-1.91**			**90**
1-chloronaphthalene	90-13-1	0.67	0.25	0.42	15349
Dichloronaphthalene	2198-77-8	1.34	0.50	0.84	1648
Trichloronaphthalene	1321-65-9	1.57	0.67	0.90	724
Tetrachloronaphthalene	1385-882	1.74	0.79	0.95	317
Pentachloronaphthalene	1321-64-8	1.85	0.88	0.97	160
Hexachloronaphthalene	1335-87-1	1.91	0.93	0.98	90
Heptachloronaphthalene	32241-08-0	1.90	0.96	0.94	107
Octochloronaphthalene	2234-13-1	1.90	0.98	0.92	105
Short chain chlorinated paraffins (SCCPs)	**85535-84-8**	**0.02-1.79**			**255**
Monochloro-octane	628-61-5	0.01	0.00	0.00	60286
Monochloro-nonane	2473-01-0	0.02	0.01	0.02	55889
Monochloro-decane (20% w/w Cl)	1002-69-3	0.07	0.00	0.07	48759
Dichloro-octane	2162-99-4	0.10	0.09	0.01	45078
Dichloro-nonane	821-99-8	0.14	0.10	0.04	40959
Dichloro-dodecane	3922-28-9	1.16	0.43	0.74	2693
Hexachloro-decane (61% w/w Cl)	51990-12-6	1.79	0.89	0.90	~255
Perchloro-decane (87% w/w Cl)		1.00	1.00	0.00	~4088
Ugilecs					
TCBT (Ugilec 141)		**1.86**	0.88	0.97	**157**
DCBT (Ugilec 121, Ugilec C21)		**1.61**	0.67	0.94	**610**
2,2'-methylenebis(3-chlorotoluene)	84604-92-2	1.67	0.73	0.94	499
2,2'-methylenebis(4-chlorotoluene)	84604-91-1	1.67	0.73	0.94	500
Commercial Pentabromodiphenyl ether*:		**1.83-1.86**			**185**
2,2',4,4'-tetraBDE (BDE-47)	40088-47-9	1.83	0.88	0.95	185
2,2',4,4',5-pentaBDE (BDE-99)	32534-81-9	1.86	0.94	0.93	140
Commercial Octabromodiphenyl ether:**		**0.99-1.40**			**1379**
2,2',4,4',5,5'-hexaBDE (BDE-153)	68631-49-2	n.a.			n.a.
2,2',4,4',5,6'-hexaBDE (BDE-154)	207122-15-4	n.a.			n.a.
2,2',3,3',4,5'-hexaBDE	36483-60-0	1.40	0.96	0.44	1379
2,2',3,3',4,5',6 heptaBDE (BDE-175)	446255-22-7	n.a.			n.a.
2,2',3,4,4',5',6-heptaBDE (BDE-183)	207122-16-5	n.a.			n.a.
2,2',3,3',4,5,6-heptaBDE	68928-80-3	0.99	0.98	0.01	4776
2,2',3,3',4,4',5,5'-OctaBDE	32536-52-0	0.99	0.99	0.00	4711
Polychlorinated biphenyls (PCBs)		**1.82-1.95**			**34**
Heptachlorobiphenyl (PCB 173)	28655-71-2	1.82	0.97	0.86	202
Pentachlorobiphenyl (PCB 116)	25429-29-2	1.89	0.90	0.99	118
Hexachlorobiphenyl (PCB 155)	33979-03-2	1.92	0.93	0.98	81
Decachlorobiphenyl (PCB 209)	2051-24-3	1.95	0.99	0.96	34

Table cont'd on next page

Polychlorinated dibenzodioxins (PCDDs)		**1.68-1,77**			**287**
2,2',3,4,4',5-hexachloro dibenzodioxin	34465-46-8	1.68	0.96	0.88	462
2,2',3,3'-tetrachloro dibenzodioxin (TCDD)	1746-01-6	1.77	0.88	0.90	287
Polychlorinated dibenzofurans (PCDFs)		**1.43-1.80**			**247**
2,4,4'-trichlorodibenzofuran	54589-71-8	1.43	0.73	0.70	1208
2,3,4,4',5,5'-hexachlorodibenzofuran	55684-94-1	1.80	0.94	0.85	247
Polyaromatic hydrocarbons (PAHs), a.o.:		**0.16-1.48**			**993**
Naphthalene	91-20-3	0.16	0.00	0.16	39675
fluorene	86-73-7	0.50	0.22	0.29	21175
Acenaphthylene	208-96-8	0.57	0.15	0.43	18522
anthracene	120-12-7	1.15	0.58	0.57	2799
Phenanthrene	85-01-8	1.17	0.58	0.58	2662
benz[b]fluoranthene	205-99-2	1.41	0.79	0.62	1358
fluoranthene	206-44-0	1.41	0.74	0.67	1332
benz[k]fluoranthene	207-08-9	1.43	0.79	0.64	1221
Chrysene	218-01-9	1.48	0.77	0.71	995
benz[a]anthracene	56-55-3	1.48	0.77	0.71	993

* Commercial pentaBDE is listed in the Stockholm convention as follows: 'Tetrabromodiphenyl ether and pentabromodiphenyl ether means 2,2',4,4'-tetrabromodiphenyl ether (BDE-47, CAS No: 5436-43-1) and 2,2',4,4',5-pentabromodiphenyl ether (BDE-99, CAS No: 60348-60-9) and other tetra- and pentabromodiphenyl ethers present in commercial pentabromodiphenyl ether.'

** Commercial octaBDE is listed in the Stockholm convention as follows: 'Hexabromodiphenyl ether and heptabromodiphenyl ether mean 2,2',4,4',5,5'-hexabromodiphenyl ether (BDE-153, CAS No: 68631-49- 2), 2,2',4,4',5,6'-hexabromodiphenyl ether (BDE-154, CAS No: 207122- 15-4), 2,2',3,3',4,5',6-heptabromodiphenyl ether (BDE-175, CAS No: 446255-22-7), 2,2',3,4,4',5',6-heptabromodiphenyl ether (BDE-183, CAS No: 207122-16-5) and other hexa- and heptabromodiphenyl ethers present in commercial octabromodiphenyl ether.'

The approach used in Table 9, where the various constituents are checked for their PB-score, can be followed for any (commercially available) mixture, However, for nomination purposes it should always be checked if the (high scoring) components are present in the mixture in quantities that are relevant for the regulatory framework under consideration.

DDT in Dicofol

Dicofol, nominated by the Netherlands for inclusion in the UNECE LRTAP POP protocol, contains the confirmed POP DDT. For the purpose of this exercise it is assumed that DDT is present in relevant quantities, In this case, DDT scores 1.92 and Dicofol scores 1.89 (Table 9), indicating that both substances fulfil the P and B criteria.

Commercial Octabromodiphenyl ether

For commercial octabromodiphenylether none of the specific components mentioned in the Stockholm convention (see the second footnote under Table 9) is present in our list of 64.721 pre-calculated substances. OctaBDE itself, CAS 32536-52-0, has a PB-score of 0.99, with a B-score of 0.00. The substance is calculated to be very persistent (P-score 0.99), but not bioaccumulative at all. This is due to the fact that the octanol-water partition coefficient (log K_{ow}) is calculated to be very high, 10.3. The BCF_{max} based on this very high log K_{ow} is calculated to be 103, which in terms of the B-score effectively becomes 0. Indeed, for the commercial octabromodiphenyl ether technical mixture, not the octabromo- congeners itself, but more specifically

the hexa- and heptabromo congeners are considered to be bioaccumulative (see footnotes with Table 9). For the single hexa- and hepta-bromo congeners present on the list of commercially registered substances the calculated B-scores are 0.44 and 0.01 respectively. Especially the hepta-bromodiphenyl ether is not expected to be bioaccumulative according to its calculated properties, again due to the extremely high log K_{ow} of 9.44. The very low octanol-air partitioning coefficient (K_{aw}) of the higher chlorinated diphenyl ethers also suggests that no trophic magnification for air-breathing mammals will occur.

Commercial Pentabromodiphenyl ether

The two components explicitly mentioned in the Stockholm convention for commercial pentabromodiphenyl ether were both present on the EINECS list. High B-scores, and subsequently also high PB-scores, are calculated for the less hydrophobic tetra- and pentabromo-congeners with B-scores of 0.95 and 0.93.

PCNs

Commercial polychlorinated naphthalenes (PCNs) are mixtures of up to 75 chlorinated naphthalene congeners plus by-products and are often described by the total fraction of chlorine. One congener, a tetrachloronaphthalene, is shown as an example in Figure 6.

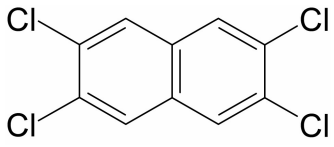


Figure 6. 2,3,6,7-tetrachloronaphthalene.

The PCN hexachloronaphthalene gives the highest calculated PB-score of the evaluated PCNs. Assuming that commercial mixtures will contain a small but relevant fraction of hexachloronaphthalene congeners, these mixtures can be characterized by this highest PB-score, 1.91, ranking place 90 of the 64.721 evaluated substances.

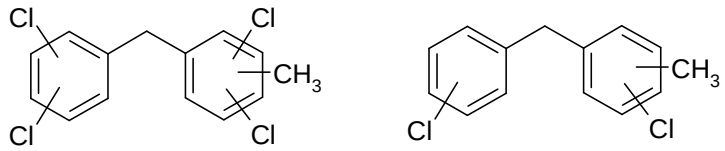
SCCPs

Short-chain chlorinated paraffins (SCCPs) are a complex mixture (UVCB). Initially (looking up the CAS-RN used for SCCPs in the list of existing substances calculated under 3.1), a very low PB-score was noted for SCCP. However, the structure assigned to the CAS number in this study was a monochlorinated *n*-decane. This structure is, however, not representative of the complex mixture of SCCPs, which contains 40-70% chlorine atoms on weight basis, while the monochlorodecane structure only has 20% w/w Cl. The commercial SCCP mixture which is stated to have an average chlorination of 60% w/w Cl would be better represented by e.g. hexachlorodecane, which has 61% chlorine atoms w/w. P- and B-scores for this substance have manually been calculated to be 0.89 and 0.90 respectively, giving a PB-score of 1.79, which would rank around place 255. The highest chlorinated SCCP, represented by perchlorodecane would give a P-score of 1.00 and a B-score of 0.00. This low B-score is due to the extremely high log K_{ow} of 16.78 which was calculated for perchlorodecane. Perchlorodecane would rank around place 4088 in the list of existing substances, next to a substance like Perfluorotributylamine, CAS 311-89-7, which is also calculated to be completely persistent, but non-bioaccumulating due to its very high (calculated) octanol-water partition coefficient. In order to calculate the highest PB-score for any component of the commercial SCCP–score, all components C8-C12 with varying chlorination from 40-70% would have to be calculated separately. Several chloro-alkanes which were present in the list of 64.721 substances evaluated in this exercise are listed in Table 9 for illustration. It is thought

that for this exercise the high POP potential of SCCPs is represented sufficiently by hexachlorodecane.

Ugilecs

Ugilecs are commercial mixtures of tetrachlorobenzyltoluenes (TCBTs, UGILEC 141) and dichlorobenzyltoluenes (DCBTs, UGILEC 121 and UGILEC C21). The TCBTs are a group of 96 individual isomers of dichlorobenzyldichlorotoluenes, with a molecular formula of $C_{14}H_{12}Cl_4$ and their general structure is presented in Figure 7. The molecular formula for the dichlorobenzyltoluenes is $C_{14}H_{14}Cl_2$, and their general structure is also shown in Figure 7. For the calculation of the PB-score, the site of chlorination is not very influential.



TCBT DCBT

Figure 7. General structure of the tetrachlorobenzyltoluenes (TCBT, Ugilec 141) and dichlorobenzyltoluenes (DCBT, Ugilec 121, Ugilec C21)

CAS numbers of individual TCBTs are not known, and it is highly unlikely that these are present in the 64.721 substance dataset for which PB-scores have been automatically generated. Instead of calculating one PB-score for Ugilecs, separate PB-scores for TCBT and DCBT are shown in Table 7, where TCBT is represented by 6-(3,4-dichlorobenzyl)-3,4-dichlorotoluene, and DCBT by 6-(3-chlorobenzyl)-3-chlorotoluene. The results are listed in Table 9. As mentioned, the exact substitution pattern of TCBT or DCBT does influence the calculated PB-score slightly, but these variations are not thought to be significant. DCBT has a calculated PB-score of 1.61, as compared to the PB-score of 1.86 for TCBT. This lower score is due to the lower persistence of the dichlorinated Ugilecs, for which an overall persistence in the environment, P_{ov}, of 311 days is calculated. The B-scores of TCBT and DCBT (0.97 and 0.94 respectively) indicate very similar bioaccumulative properties of these Ugilecs. Furthermore, two substances which were very close structural analogues to DCBT were present in the precalculated list of 64.721 substances. Formally, these can not be considered dichlorobenzyltoluenes, but dichlorotolyltoluenes, having a methyl substituent on both phenyl rings instead of on only one. Their calculated PB-scores have been included in Table 9 nevertheless. As these substances were present on the EINECS list, there might be some commercial interest.

PCTs, PCBs, PAHs, PCDDs and PCDFs

Several congeners of these mixtures can already be found in the list of 250 substances with the highest PB-scores, discussed in section 3.1 and presented in Appendix 4. These congeners can be used as representative structures for these groups, taking into account that these are the worst-case POP characteristics, and it has to be confirmed that this specific congener is present in a commercial mixture in relevant quantities if the PB properties of this single representative structure are to be used to describe the commercial mixture. Several components for each POP mixture are listed in Table 9.

For PAHs it is thought that the 16 PAHs selected by the US EPA, and for which a number of PB-scores are listed in Table 9, are representative for the whole group of PAHs. The highest scoring PAHs in this selection of 16 are chrysene and benz[a]anthracene.

3.3 PB-scores for EU PBT/vPvB substances

3.3.1 Evaluation of individual PBT/vPvB substances

Before REACH entered into force on June 2008, a EU working group on PBT substances (as part of the Technical Committee on Existing and New Substances) discussed 127 potential PBT/vPvB substances in detail, giving advice on the designation of a substance as confirmed PBT or confirmed vPvB substance. The 19 substances that were inferred to be PBT or vPvB are listed in Table 10 together with their estimated P-, B- and combined PB-score.

DDT, Lindane, hexachlorobutadiene and *hexachlorobenzene* have already been discussed in section 3.2.1. *Dicofol, endosulfan, octabromodiphenyl,* and *hexabromocyclododecane* are discussed in section 3.2.2. For a discussion of *SCCPs* and *PAHs* see section 3.2.3

For the two *trichlorobenzenes* on the list the PBT criteria were marginally met. P-scores of 0.45-0.46 are indicative of overall half-lives close to 180 days, and the overall half-life is therefore estimated to be higher than 120 days, which is the P criterion for the compartment soil and sediment within the EU PBT framework. A BCF-value equal to the B criterion of 2000 would result in a B-score of only 0.18. Indeed, these substances do not score high for bioaccumulation, and the scores are even somewhat lower than 0.18. Given the fact that the reliable experimental BCF-values are all below 2000, the estimated B-scores are well in accordance with the experimental values.

Cyclododecane was inferred to be PBT and vPvB based only on screening data for persistence and toxicity. These screening data included ready biodegradability test results for persistence and only QSAR information for toxicity. The substance showed some degradation in the ready biodegradability test, and the lack of passing the ready biodegradability criteria might be due to reduced bioavailability. However, the very low P-score of 0.02 in Table 8 seems to be a result of overestimating the biodegradability. The B criterion was clearly met with a BCF-value of 13700. The B-score of 0.40 is lower than expected from the BCF, which suggest that metabolism (as well as biodegradability) is overestimated by the model for this substance.

Nitrofen has a rather high PB-score of 1.56. This is in accordance with its assignment as PBT substance. Nevertheless, the PBT assessment was based only on screening data for persistence and toxicity. The bioaccumulation potential was deduced from non-standardized tests in a model ecosystem study. Nitrofen was inferred to be B (BCF>2000), but not vB (BCF>5000). The BAF for aquatic organisms was estimated to be only 1783, which is close to the B criterion of 2000. The high B-score (0.75) is partly due to the potentially high biomagnification in air-breathing organisms (TMF of 9.2).

Pentachlorobenzenthiol was inferred to be PBT and vPvB based on screening data, with no experimental data on bioaccumulation and toxicity, and only ready biodegradability results for persistence. Nevertheless, the PB-score is in agreement with this PBT and vPvB status.

Table 10 Confirmed PBT and vPvB substances from EU existing substances (EINECS)

Substance	CAS RN	PB-score	P-score	B-score	Rank
DDT	50-29-3	1.92	0.94	0.98	82
Dicofol	115-32-2	1.89	0.95	0.94	109
Hexachlorobenzene	118-7-1	1.85	0.92	0.93	170
SCCPs [a]	85535-84-8	1.79	0.89	0.90	255
Pentachlorobenzenethiol	133-49-3	1.77	0.87	0.90	289
Hexabromocyclododecane [b]	25637-99-4	1.68	0.74	0.94	~470
Lindane	58-89-9	1.67	0.87	0.80	484
Nitrofen	1836-75-5	1.56	0.75	0.81	742
Coal tar pitch UVCBs [c]	--	1.48	0.77	0.71	995
Octabromodiphenylether [d]	32536-52-0	1.40	0.96	0.44	1.379
Endosulfan	115-29-7	1.35	0.89	0.47	1.577
Hexachlorobutadiene	87-68-3	1.32	0.85	0.46	1.751
Anthracene and anthracene containing UVCBs [c,e]	120-12-7	1.15	0.58	0.57	2.799
Musk xylene	81-15-2	0.84	0.84	*0.00* [g]	9.679
1,2,3-trichorobenzene	87-61-6	0.60	0.46	*0.14*	17.594
Bis(tributyltin)oxide and tetrabutyltin [f]	56-35-9	0.58	*0.00*	0.58	18.359
1,2,4-trichlorobenzene	120-82-1	0.51	0.45	*0.06*	21.039
Cyclododecane	294-62-2	0.42	*0.02*	0.40	24.440
Tetramethyllead	75-74-1	0.05	*0.05*	*0.00*	51.588

[a] Scores given for representative structure hexachlorodecane, see Table 9.

[b] Scores given for representative structure 1,2,5,6,9,10-HBCDD, see Table 8.

[c] Both P- and B-score above 0.5 for anthracene, phenanthrene, fluoranthene, benz[*a*]anthracene and chrysene, benzo[*b*]fluoranthene, and benzo[*k*]fluoranthene. Highest scores given here are for benz[*a*]anthracene. See Table 9.

[d] For a discussion on (commercial) Octabromodiphenylether see section 3.2.3 and Table 9.

[e] Scores given for anthracene.

[f] Tetrabutyltin contains tributyltin and degrades to bis(tributyl)tinoxide (TBTO) in the environment.

[g] P- or B-scores indicated in *italics* indicate that these scores do not comply with the assigned PBT status (see table 4).

Organometals are outside the domain of the QSAR models applied for the calculation of the P- and B-score. This could explain why the PB-scores for *tetramethyllead* and *bis(tributyltin)oxide*, two confirmed PBT substances, are very low. Only the bioaccumulation potential for bis(tributyltin)oxide is estimated fairly well.

Musk xylene, which is a confirmed vPvB substance, is predicted to be extensively metabolized in fish ($t_{1/2}$ of < 5 hours), while this is not confirmed by experimental data. Furthermore, the estimated log K_{ow}-value for musk xylene (4.45) is lower than the experimental value (4.9), thus further reducing the B-score. Its calculated BCF_{max} is 4500, but correction for (estimated) metabolism yields a BCF of 55. An estimated TMF of 2.25 (in accordance with Kelly et al. 2007) increases this BCF to a BAF of 125. In conclusion musk xylene would not be identified as potential vPvB by this method due to overestimation of metabolism.

3.3.2 Statistical evaluation of the performance of the PB-score

Another check on the performance of the PB-score methodology was made by comparing the assignment for P and B that was made in EU PBT working group on the basis of information other than QSAR estimates to the individual calculated P- and B-scores obtained in this exercise. Out of all 127 substances that were considered in the PBT working group under the Technical Committee for New and Existing Substances (TCNES) of the European Union (EU), P- and B-scores could be estimated for 98 substances. For the remaining 29 substances a single representative structure could not be assigned automatically. Out of these 98 substances, the P-status was definitively assigned to 48 substances, and for 28 substances a preliminary conclusion was drawn for P, while for the remaining 22 substances a preliminary conclusion could not be reached. Similarly, for the B-status of these 98 substances a definitive conclusion was reached for 50 substances, and for 14 substances a preliminary conclusion was drawn, while for the remaining 34 substances a preliminary conclusion could not be made. For this evaluation exercise P and vP conclusions, and B and vB conclusions were lumped together resulting in the following categories:

- confirmed non-P, P or vP (48)
- preliminary conclusion non-P, P or vP (28)
- no (preliminary) conclusion on P-status reached (22)
- confirmed non-B, B or vB (50)
- preliminary conclusion non-B, B or vB (14)
- no (preliminary) conclusion on B-status reached (34)

The number of substances in these groups was extended with the substances that have been evaluated in POP frameworks (UNEP, UNECE). Substances that meet the screening criteria for POPs (i.e. they are already POP or proposed as POP) and were not already on the list of the EU PBT Working Group were aldrin, chlordane, chlordecone, dieldrin, endrin, heptachlor, hexabromobiphenyl, mirex, PCBs, toxaphene, PAHs, dioxins/furans, PFOS, commercial pentabromo diphenyl ether, polychlorinated naphthalenes, and pentachlorobenzene. As these substances were definitively confirmed to fulfil the POP screening criteria they were added to the groups of confirmed P/vP and confirmed B/vB.
Of the remaining substances that are under consideration, trifluralin was added to the groups preliminary P/vP and preliminary B/vB, while pentachlorophenol was added to the groups preliminary non-P and preliminary non-B. The substances DDT, lindane (HCHs), hexachlorobutadiene (HCBD), endosulfan, dicofol, hexachlorobenzene, HBCDD, commercial OctaBDE, short-chain chlorinated paraffins SCCPs were already in the list of 127 substances considered by the EU PBT working group. Their assignment in the POPs framework matched that of the PBT working group.

The individual P- and B-score calculation has been compared with the conclusion on the P and/or B properties of these substances in the EU PBT working group and in the POP framework. The results of this exercise are presented in the graphs in Figure 8. The graphs show pair wise comparisons between substances without and with PBT characteristics and their calculated PB-scores (on the y-axis). There is a clear statistical difference between the groups assigned preliminary or confirmed P- or B-status (or vP or vB) and the group that was preliminary concluded or confirmed to be not B or not P.

Although the group of 127 substances was already pre-selected for the PBT working group based on their potential PBT characteristics, the statistical differences between the P- and B-scores of confirmed P/vP and confirmed non-P and between confirmed B/vB and confirmed non-B were highly significant. The difference between the substances that were considered to meet the P criterion and those that were considered not to meet the P criterion is highly significant ($P<0.0001$). Similar results were obtained for the differences between substances for which the B criterion was concluded to be fulfilled and those substances for which the B criterion was not fulfilled ($P=0.0004$). For substances for which the assignment of the P and B status was not definitive yet, the differences between the average PB-score for the groups of P/B and non-P/non-B were not significant. However, this is probably related to the low number of substances in these groups (only 4 substances with a preliminary conclusion of non-P and only 6 with a preliminary conclusion non-B).
For all subgroups, the mean score of the group considered to fulfil the criteria was higher than the mean score of the group that are considered to fail the criteria. Only for the groups of substances that were assigned preliminary conclusions on P and B, the differences between the mean scores were not significant, but this may be due to the low number of substances as well ($n=4$ for preliminary non-P and $n=6$ for preliminary non-B).

The mean P-score for the group of substances that were confirmed to fulfil the P criterion was 0.81, which refers to an overall half-life of as much as 600 days. For the group of substances that were confirmed not to meet the P criterion, the mean P-score was 0.37, which is equivalent to an overall half-life of 125 days. The mean B-score for the group of substances that were confirmed to fulfil the B criterion was 0.59, which equals a bioaccumulation factor of 6560. For the group of substances that were confirmed not to meet the B criterion, the mean B-score was 0.26, which is still equivalent to a bioaccumulation factor of 2570. The bioaccumulation factor is not directly comparable to the B criterion as it contains a trophic magnification factor in air-breathing organisms as well, while the B criterion only considers aquatic organisms.

It can be concluded that, on average, the applied methodology results in clearly different PB-scores for substances that are PBT substances and those that are not. This tool seems very useful to identify potential POP and/or PBT and vPvB substances. On the other hand, it is not meant to verify or falsify the POP or PBT characteristics of individual substances without further scrutiny of the PB-score calculation made with the tool.

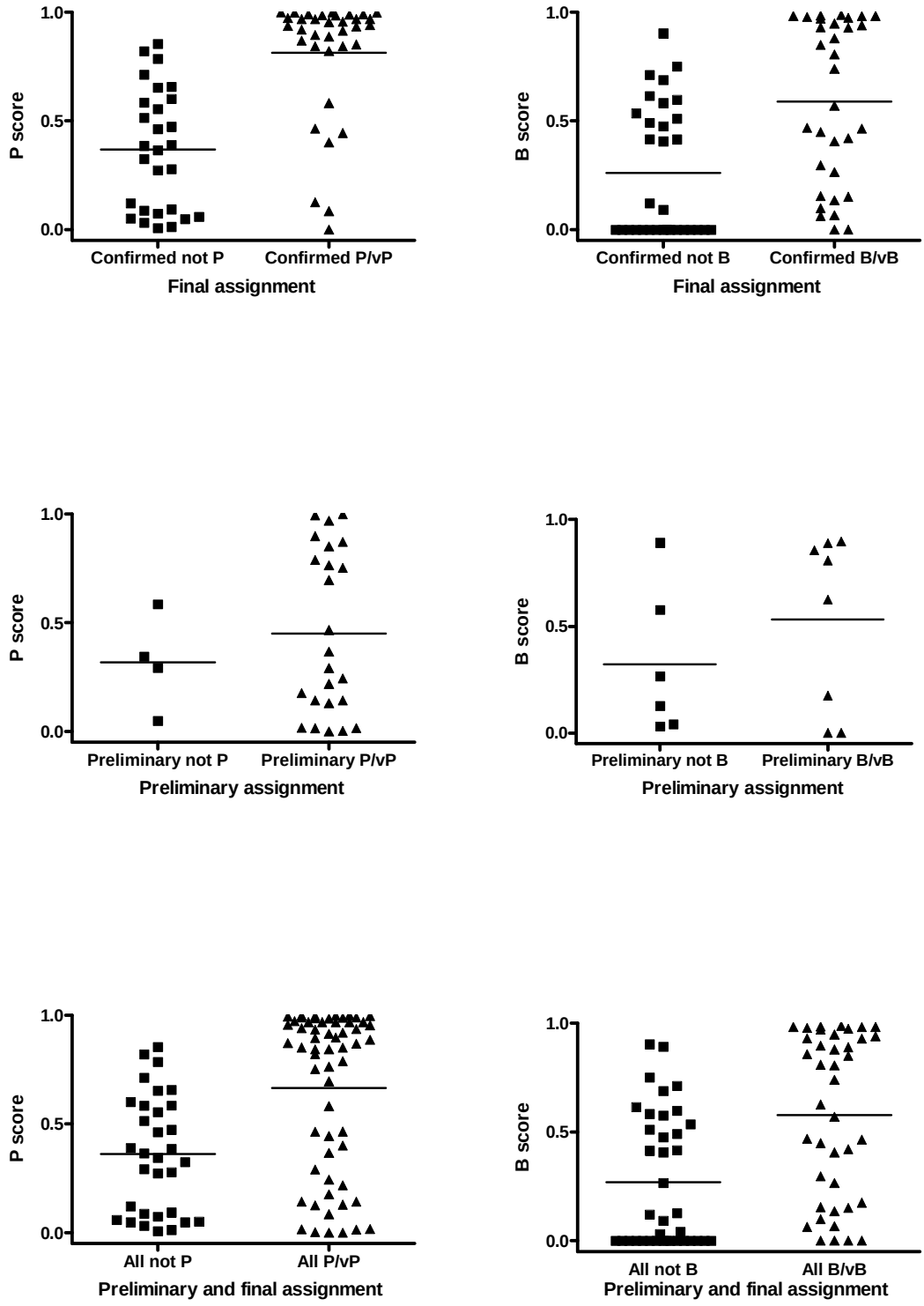


Figure 8. Statistical comparison of the calculated PB-score from substances that were concluded to fulfil the P- and B-criteria vs. substances that were concluded to not fulfil the P- and B-criteria, as discussed in the TCNES PBT working group and the TFPOP/POPRC. The horizontal line represents the average score within each group.

4 Discussion and Conclusions

In this study, a quantitative score has been developed to represent the potential P- and B-properties of a substance. The methodology allows for the addition of the scores representing the P- and B-properties, after transformation, scaling and centring of the individual P- and B-properties. Because of the similar scale of the P and B properties it is easy to assign a specific weight to these properties to come to a combined PB-score. In our exercise, we have chosen to weigh Persistence and Bioaccumulative properties equally. Any other property for which there is a need to give it a weight in a specific score can be calculated equally (transformation, scaling and centring), and the score can be added identically. In this way, toxicity could be added for screening of potential PBT properties.
The PB-score as proposed in this study is used to generate a priority list which can be used to select future potential POP or vPvB candidates. Some imperfections of the procedures followed in this study need to be taken into account when interpreting this 'priority list'.

Absence of metabolites, impurities and byproducts in a final priority list
The newly developed PB-score has been applied to a large number of substances, in order to determine which (kinds of) substances score very high, and may be future potential POP, vPvB or PBT candidates. The PB-score was generated automatically by batch processing lists of commercial substances represented by their CAS numbers. Structure information was assigned to these CAS numbers and this structure information was used in a number of QSARs to estimate the P- and B-properties. This automatic procedure, based on lists of commercial substances has some inherent drawbacks.

1. The lack of (persistent) degradation products. Good examples in this study are the anisoles, as degradation products of phenols. Specifically pentachloroanisole is a potential substance of concern, but as it has no commercial application, it was absent on any of the lists used for calculation of the PB-scores. Therefore, in a list of very high scoring substances (such as presented in Appendix 4) pentachloroanisole is not present.
2. The lack of impurities and byproducts. In a similar way as the degradation products, impurities and byproducts which can be substances of concern themselves, might not be present in the list of top-scoring substances, as they are not (always) present on the lists used in this study to generate PB substances. Examples of such substances which are present as impurities in commercial products are the polychlorinated dibenzodioxins and dibenzofurans.

Absence of mixtures and natural products in a final priority list
Another omission in the list of top-scoring substances generated in this study is the absence of mixtures and natural substances, as these often do not have a representative chemical structure assigned to their CAS registration number. Examples are commercial Aroclor mixtures, which are present on the EINECS list, whereas the individual PCB-congeners, of which the Aroclor commercial products are made up, might not all be present on the EINECS list of existing substances. Another example, which has been touched upon in the results section (section 3.2.3), relates to the short chain chlorinated paraffins (SCCP). The CAS-RN for the (commercial) product is present on the EINECS list used for generation of the PB-scores. However, the 'representative' chemical structure that was assigned to SCCP in the CAS-chemical structure lists, turned out not to be the right representative structure for

this specific purpose of calculating the (highest) PB-score of a mixture. Therefore, SCCP initially ended up at the very bottom in the ranking based on PB-scores (with PB-score of 0.07).

The difficulties described above are strongly related with the choice to use databases on commercial products as input. These databases are easy to obtain and a further consideration was that any measures following the assignment of a substance as a PBT or POP candidate has to focus on commercial products. A systematic approach to overcome the problems described above would be to include databases on individual substances including metabolites, by-products, to calculate a PB-score for each individual component of mixtures and natural products and to select the highest scoring component to represent the mixture. An option to do this in an automated way would be to use the information presented in the publicly available PubChem database, which is organized in such a way that it would be possible to split each 'substance' into separate 'components' which each have a single chemical structure, suitable for calculation of a PB-score.

Weight of P and B properties in an overall PB-score

The 'weighting' of the different properties taken into account in a score (in this case Persistence and Bioaccumulation) is a subjective part of the newly developed P- and B-scores. This is not only influenced by the individual weight of the scores (in this study P- and B-scores are given identical weight), but is influenced heavily also by the choice of the value used to centre the individual score. The P-score has been centred on an overall persistence, P_{ov}, of 180 days. It could, however, also be argued that 120 days would have been a valid choice, since a maximum aquatic half-life of 60 days (vP-criterion) would automatically lead to a (estimated) soil half-life of 120 days, not 180 days (vP-criterion). When the P-score is centred on a P_{ov} of 120 days instead of 180 days, the 'weight' of Persistence in relation to Bioaccumulation will become higher. The same holds true in reverse, when centring of the B-score is performed around a BAF of 2000 (B criterion) instead of 5000 (vB and POP criterion). The choice of individual property 'weight' will therefore also be very dependent on the regulatory framework for which the PB-score is needed. The PB-score as used in this study is tailored for the identification of POP and vPvB substances. For identification of PBT substances, a T criterion needs to be added, and the weights of the P- and B-criteria (and their cut-off values used for centring) need to be re-established.

It should be noted that the influence of the centring is probably minimal when the goal of the exercise is to generate a list of top-scoring substances selected for further investigation. However, when the score is used as a quick way to determine whether a substance would meet the POP or vPvB criteria, the choice of weight and centre becomes crucial. An objective way to weight individual properties which are combined into one score is called 'swing weighting' [Clemen, 2006], which might be applied in an update or extension of this methodology, especially when more properties (e.g. Toxicity) are going to be combined into one score. Toxicity and long-range transport may be added to the score in future exercises, but it should be taken into account that these characteristics partly correlate with toxicity and persistence (see chapter 2.2) and that interpretation of the combined score becomes more complicated.

Evaluation of the PB-score performance using confirmed POPs

The newly developed PB-score seems to reflect the concern that leads to inclusion of substances into the POP conventions, and might therefore serve to select candidates for nomination of new substances for these conventions. In fact, only one POP substance or nomination scored markedly below the POP criteria. This was hexabromobiphenyl, which had a calculated B-score of 0, due to the fact that its

calculated octanol-water partition coefficient is extremely high. A different estimation programme for log K_{ow} (ClogP) would have given a much higher PB-score for this substance. Octabromodiphenylether exhibited similar characteristics. In the nomination process for the UNEP Stockholm Convention the hepta- and hexaBDE congeners were nominated as representatives for commercial OctaBDE, as it was recognized that octaBDE itself did not meet with the criteria (see also tables in chapter 3.2.1 and 3.2.2).
One substance, trifluralin, was calculated to only marginally bioaccumulate (B-score of 0.15), which could be attributed to the estimated very short metabolism half-life (0.6 days). Within the UNECE TFPOP it was put forward that model estimations and experimental data provided relatively high BCFs, but that high levels were hardly observed in the field.

Overall, it can be concluded that this newly developed PB-score gives a very good first indication of the potential POP behaviour of a chemical substance.

Evaluation of the PB-score performance using EU PBT candidates
Calculated P- and B-scores were compared to the designation of P and/or B properties for substances discussed in the PBT working group (TC-NES). All substances discussed in the PBT working group were already considered to be potential PBT substances. Therefore, the selectivity of the P- and B-score shown for this pre-selected group of potential PBT substances is probably much better when applied to substances which have not been pre-selected on the basis of their potential PBT properties. The final conclusion on the P- and B-status of the substances is reached based on experimental data.
It must be stressed that, although the average values are clearly higher for substances that are considered P or B, individual assessments may be far off. For several substances that were considered to meet the P or B criterion, the respective P- or B-score was close to zero. For persistence this may be due to the fact that the estimation programme is not suitable for the specific subgroup (e.g. organometals) or that the substance may be persistent in several compartments, but is so effectively transported to other compartments where degradation is relatively fast, that the overall persistence is low (e.g. methylcyclosiloxanes). These findings show that the method can still be improved, and that for nomination of substances as a PBT or POP candidate the model estimations should be confirmed by experimental data.

Quantitative nature and margin of error of the PB-score
The estimation of properties, purely based on chemical structure and automated for large numbers of chemically very diverse substances, yields the risk that a large margin of error may be present in the calculated scores. The precision suggested by the quantitative nature of the PB-score does not mean that one can fully interpret the score quantitatively. The quantitative nature of the method, however, does allow us to rank substances according to this score, and should allow distinguishing the substances with low potential for POP or vP/vB properties from substances with high potential. Although the score cannot be interpreted as an absolute value, based on the validation using existing and proposed POPs and potential PBT/vPvB substances, we do think that the newly developed PB-score can be used for priority setting in the context of POP and PBT/vPvB regulations.

Further perspectives
Building a priority setting methodology and carrying out the actual ranking brought various problems to light that had to be tackled. Some of the problems have been mentioned in the previous sections and have been solved in the present study. For other problems, possible solutions have been proposed, but have not yet been

implemented and may be solved in future projects, for example how to best address the PB-score of mixtures and how to tackle and incorporate metabolites. Adding toxicity and long range transport potential to the combined score can be considered as well, as indicated above.

This study was started to identify substances for further investigation that are promising for nomination as potential POP or vPvB/PBT substances in the (near) future. The current results, as included in chapter 3 (Table 5) and Appendix 4 are considered to be a first step to identification of such substances. In the second step, experimental data have to be gathered on persistence, bioaccumulation, toxicity and long-range transport to substantiate or negate the concerns for the substances that are identified. From a policy perspective, other considerations come into play as well. such as marketing volume, wide dispersive use and socio-economic considerations. The interplay between scientific considerations and policy objectives will determine which substances may be addressed in follow-up work to the current study.

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Appendix 1: Previous studies on the selection of POPs and PBTs

Dutch ministry of Housing, Physical planning and the Environment DGM – BKH Consulting

In 1997, BKH Consulting Engineers performed a selection of toxic, persistent and bioaccumulative substances for the Dutch ministry of Housing, Physical planning and the Environment DGM/VWS (Blok et al., 1997). All 180.000 substances from the ISIS/Riskline database were taken into account, for which aquatic toxicity data were collected. Those data were available only for 3600 substances. From this subset, only organic substances were selected with a LC50 < 1 mg.l-1 or NOEC < 0.1 mg.l-1, and for which a SMILES notation could be derived. 639 Compounds remained. These compounds were screened for their bioaccumulation potential and biodegradability following the criteria:

persistence:	Probability for rapid degradation < 0.1 (Syracuse BIODEG) or atmospheric $t_{1/2}$ < 2 days for substances that distribute to atmosphere for more than 10% (Mackay level I model);
bioaccumulation:	log K_{ow} > 4 (KowWin) or BCF > 1000;

Based on these selection criteria, 54 substances were identified as PBTs.

COMMPS/Water Framework Directive

In 1999, the Fraunhofer Institut elaborated a combined monitoring-based and modelling-based priority setting scheme (COMMPS) in order to establish a list of priority substances in the context of the Water Framework Directive (WFD; Klein et al., 1999). Candidate substances were selected from various official substance lists and monitoring programmes: i) List I and II of Council Directive 76/464/EEC, ii) Annex 1a and 1d of the 3rd North Sea Conference, iii) Priority lists 1-3 under Council Regulation 793/93, iv) OSPAR list of individual candidate substances, v) HELCOM list of priority substances, vi) pesticides under Council Directive 91/414/EEC, vii) monitored substances, together resulting in a selection of 658 substances. Next, the substances were ranked according to their aquatic exposure scores, i) based on surface water monitoring data and ii) based on fugacity modelling data. Effect score rankings were established based on test data, and a risk-based score was given to each substance by multiplying exposure and effect scores. From these risk scores, a final recommendation of priority substances in the context of the WFD was made based on, substance-by-substance, expert judgment. 32 Substances were selected as high priority substances.

In a report of the European Commission of 2001 on the identification of priority hazardous substances in the context of the WFD, the COMMPS procedure and the proposed list of priority substances was still applied without any modification or change as the first selection criterion for POP-like substances (European Commission, 2001).

OSPAR studies

In 2001, Ökopol Hamburg (Heitman and Ahrens, 2001), on behalf of the OSPAR Commission and WWF prepared a report on 42 chemical substances that were i) suspected to have a PBT profile, ii) that were produced in relevant amounts on the European market, and iii) that may be of concern for the marine environment. In that study, a first selection of substances was performed by an ad hoc working group under OSPAR based on the DYNAMEC Mechanism. Substances were selected that potentially have PBT properties with regard to the marine environment following a number of criteria:

persistence:	half-life in water > 50 to 60 days or not inherently biodegradable;
bioaccumulation:	bioconcentration factor > 500;
toxicity:	aquatic toxicity < 1 mg.l-1 or CMR substance.

An update of the cut-off values for the selection criteria of the OSPAR Dynamic Selection and Prioritization Mechanism for Hazardous Substances was given in 2005 (OSPAR, 2005; 2006). In those studies, identical selection criteria were used as for the first selection in the study of Ökopol Hamburg, with the addition of log K_{ow} > 4 as a second indicator of the liability to bioaccumulate. In the 2001 study, those substances were treated that were obviously on the European market, resulting in a selection of 42 substances. Companies producing these substances were asked to provide information on emissions and marine exposures, on which a final selection of substances of concern was based.

Swedish EPA/Swedish National Chemicals Inspectorate (KemI)
In 2002, on behalf of the Swedish government, the Swedish Environmental Protection Agency (EPA) and the National Chemicals Inspectorate (KemI) performed a priority study on substances fulfilling the criteria for POPs set up by the Stockholm Convention and the UNECE-LRTAP Convention on persistent organic pollutants (KemI/EPA, 2002). The study was performed for substances selected or reviewed by i) the LRTAP Convention working groups, ii) OSPAR, iii) the EU programmes for new and existing substances (67/548/EEC and 793/93/EEC), iv) plant protection products from 91/414/EEC, v) classification and labelling, vi) the HELCOM list of substances, vii) the EU water directives (76/464, WFD 2000/60/EC) and vii) the Swedish 'begränsningslistan'. The criteria they employed for selecting potential POPs were:

persistence:	half-life in water > 2 months or in soil/sediment > 6 months;
bioaccumulation:	bioconcentration factor > 5000, if not available log K_{ow} > 5;
toxicity:	case by case assessment;
long-range transport:	presence of substances in remote areas or half-life in air > 2 days and volatility < 1000 Pa.

The substances that were reviewed were classified into 5 groups ranging from highest to lower priority substances.

Danish EPA
In 2002, the Danish EPA made a screening of potential PBTs and vPvBs according to the principles of the EU TGD for all organic substances that were on the EINECS list (about 50.000 substances). QSAR models were applied to estimate biodegradation rates, bioaccumulation and toxicity to mammals and aquatic species. Criteria applied for the identification of PBT and vPvB substances were:

PBT criteria:

persistence:	Half-life > 60 d in marine water, or in freshwater > 40 d, or in marine sediment > 180 d, or in freshwater sediment > 120 d (based on BIOWIN and MITIDEG);
bioaccumulation:	BCF > 2000 (based on BCFWIN and BCFConnell);
toxicity:	Chronic NOEC < 0.01 mg/l or CMR or endocrine disrupting effects (based on various sources).

vPvB criteria:

persistence:	Half-life > 60 d marine or freshwater, or >180 d in marine or fresh water sediment (based on BIOWIN and MITIDEG);
bioaccumulation:	BCF > 5000 (based on BCFWIN and BCFConnell, version….).

Also, a preliminary environmental release and exposure scoring of the selected substances was included. The performed QSAR exercise on selection of potential vPvB/PBTs indicated that the number of potential vPvB and PBT with a production volume in the EU countries greater than 10 tpa per manufacturer is 134, of which 66 were registered as used in chemical products on the Nordic market.

USEPA PBT Profiler

The EPA has developed a so-called 'PBT Profiler' which can estimate the persistence, bioaccumulation and aquatic toxicity of a substance on the basis of the molecular structure. This web-based PBT Profiler was initially developed as part of the 'P2 framework' which, in the absence of experimental data, allows OPPT (EPA Office of Pollution Prevention and Toxics) to screen substances at an early stage of R & D for undesirable traits. In fact, it can be used by different parties to quickly get information about the potential characteristics of a PBT substance. For determining whether a substance is persistent, bioaccumulative and toxic, the EPA uses the following criteria:

Table A5. Criteria for determining persistence, bioaccumulation and aquatic toxicity as used by the EPA

Property	**Criterion**
Persistent	T½ > 60 days in water, soil and sediment T½ > 2 days in air
Very Persistent	T½ > 180 dagen in water, soil and sediment
Bioaccumulative	BCF > 1.000 L/kg
Very Bioaccumulative	BCF > 5.000 L/kg
Low toxicological concern	NOEC fish > 10 mg/l
Moderate toxicological concern	NOEC fish > 0,1 - 10 mg/l

Instrument

The user can enter a substance with a unique identification: CAS number, product ID or acronym. Through a computerized search in an existing database of 100,000 compounds a SMILES notation is generated. The SMILES notation can be entered directly or generated by drawing a structural formula.

The structure of the substance then passes to nine independent modules (QSARs) to estimate the physical/chemical properties. The results are translated into a persistence, bioaccumulation and toxicity value and compared with the EPA criteria. If a substance meets the PBT criteria, the potential PBT properties of the substance should be further investigated.

PBT strategies typically focus on the persistence of a chemical in water, soil, or sediment, because bioaccumulation occurs in these media. The PBT Profiler determines how the substance is first divided among the various media (expressed as a percentage of the total volume in the environment) using a (Level III) multimedia mass balance model. Then, it is determined in which of these three compartments the chemical is most likely to accumulate (the one with the highest percentage). Subsequently, the half-life in this compartment is compared with the EPA criteria. If the half-life in the predominant compartment exceeds the EPA criteria, the chemical is designated as persistent or very persistent. However, the persistence in a specific compartment is not considered relevant if the modelling shows that partitioning of the substance to this compartment can not be expected. This helps to take into account two major components: the removal and the partitioning of the substance in the environment.

The bioaccumulation potential is directly inferred from an estimated bioconcentration factor (BCF). The BCF is estimated using the SRC BCFWIN estimation programme, based on K_{ow} and one or more correction factors based on chemical structure, if applicable. The current version of the model also takes metabolism into account.

For toxicity, the PBT Profiler only takes the chronic toxicity of fish into account, which is estimated using the programme ECOSAR. This programme predicts the toxicity for algae, daphnia and fish based on structure activity relationships (SARs). In the case that toxicity using the QSAR can not be estimated this will be displayed by the PBT Profiler.

The PBT Profiler was evaluated for the 64 known PBTs of the EPA and 12 POPS of UNEP. Of the 64 EPA-PBT 's 49 were labelled as PBT substances and 13 were labelled as persistent and bioaccumulative with an incalculable toxicity. Similar results were obtained for the 12 UNEP POPS.

Not all substances can be screened by the PBT Profiler. No reliable estimates are expected for the following substance groups:

- inorganic substances;
- metallo-organic compounds;
- reactive substances (including substances that rapidly hydrolyze);
- salts;
- substances with a high molecular weight;
- substances of unknown or variable composition;
- mixtures;
- surfactants;
- highly fluorinated compounds.

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Appendix 2: Description of various estimation programmes (in Dutch)

Long range transport

Aopwin v1.92

Doel: Dit programma berekent de afbraak in de atmosfeer van organische stoffen ten gevolge van reactie met hydroxyl radicalen of ozon.
Van belang voor: de halfwaardetijd in lucht en dus voor het criterium LRT.
Criterium: halfwaardetijd groter dan 2 d.
Prioritering: Hoe hoger de halfwaardetijd, hoe hoger de prioritering.
Aantekening: Mogelijk is het deel van de stof dat geadsorbeerd is aan deeltjes in de lucht niet beschikbaar voor afbraak. Hier licht een link met de dampdruk en de Henry coëfficiënt. Verder is de afbraaksnelheid afhankelijk van de concentratie hydroxyl radicalen. Aopwin gebruikt een hydroxyl radicaal concentratie van $1{,}5 \cdot 10^6$ OH/cm3 met de aanname dat deze er alleen overdag zijn, waarbij de dag op 12 uur wordt gesteld. De halfwaardetijd in uur die wordt gegeven gaat uit van de afbraaksnelheid overdag. De halfwaardetijd in dagen neemt mee dat de stof 's nachts nauwelijks wordt afgebroken. In de REACH guidance (R.16.4.4.3) wordt uitgegaan van een gemiddelde hydroxyl radicaal concentratie over een etmaal van 5·105 OH/cm3. Met andere woorden de halfwaardetijd volgens REACH is 1,5 keer zo lang als die volgens Aopwin.

Aerowin v1.00

Doel: Dit programma berekent hoeveelheid van een stof die in lucht aan deeltjes gebonden is.
Van belang voor: de halfwaardetijd in lucht en dus voor het criterium LRT, omdat het gebonden deel niet of minder beschikbaar is voor afbraak.
Criterium: geen.
Prioritering: Hoe hoger de geadsorbeerde fractie, hoe hoger de prioritering.
Aantekening: Mogelijk is het deel van de stof dat geadsorbeerd is aan deeltjes in de lucht niet beschikbaar voor afbraak. Hier licht een link met de dampdruk en de Henry coëfficiënt.

Mpvpbp v1.43

Doel: Dit programma berekent het smeltpunt, de dampdruk en het kookpunt.
Van belang voor: dampdruk van belang voor het criterium LRT en indirect om de octanol-lucht coëfficiënt (K_{oa}) te bepalen, die van belang is voor bioaccumulatie anders dan in het aquatische milieu.
Criterium: dampdruk lager dan 2000 Pa.
Prioritering: Geen prioritering.
Aantekening: Dampdruk is ook van belang bij het bepalen van de fractie gebonden aan aerosolen.

Persistentie

Biowin v4.10

Doel: Dit programma berekent de afbraak ten gevolgde van biodegradatie door middel van 7 routines (recent is anaerobe afbraak toegevoegd).
Van belang voor: het criterium persistentie.
Criterium: halfwaardetijd hoger dan 2 maanden in water of 6 maanden in bodem of sediment.
Prioritering: Hoe lager de uitkomst van het model, hoe hoger de prioritering.

Aantekening: Biowin geeft geen directe doorvertaling naar halfwaardetijden in het milieu.In de REACH guidance wordt alleen Biowin model 2 in combinatie met met Biowin model 3 en Biowin model 6 in combinatie met Biowin model 3 als bruikbaar voor de PBT beoordeling gegeven: Biowin 2 <0.5 en Biowin 3 <2.2, of Biowin 6 <0.5 en Biowin 3 <2.2 staat voor mogelijk persistent. Biowin 2 and Biowin 6 (MITI) hebben betrekking op ready testen, Biowin 3 heeft betrekking op uiteindelijke halfwaardetijden in hter milieu. Hierbij moet worden opgemerkt dat de halfwaardetijd voor persistentie in REACH 40 dagen in zoetwater, en 120 dagen in bodem en sediment is. De halfwaardetijden in de POP-criteria komen overeen met vP onder REACH.

Hydrowin v2.00
Doel: Dit programma berekent de afbraak van organische stoffen ten gevolge van hydrolyse.
Van belang voor: het criterium persistentie.
Criterium: halfwaardetijd hoger dan 2 maanden in water of 6 maanden in bodem of sediment.
Prioritering: Hoe hoger de halfwaardetijd, hoe hoger de prioritering.
Aantekening: Niet alle stoffen zijn aan hydrolyse onderhevig. Slechts voor een aantal zal dit model een uitkomst bieden. Geen berekening betekent dus geen hydrolyse ingeschat. Het model berekent alleen zure en basische hydrolyse en zou daarmee ook een onderschatting van de hydrolyse kunnen geven.

Bioaccumulatie

KowWin v1.67 en ClogP v5
Doel: Deze programma's berekenen de octanol-water partitie coëfficiënt (K_{ow}).
Van belang voor: de hydrofobiteit, uitgedrukt als log K_{ow}, wat voor organische stoffen een belangrijke parameter is voor de potentie tot bioaccumulatie.
Criterium: log K_{ow} >5.
Prioritering: Hoogste bioaccumulatie potentiaal bij log K_{ow} van ongeveer 6.5-7 (REACH guidance Appendix R.11-1 Annex 1), dus hoe dichter bij dit gebied hoe hoger de prioritering.
Aantekening: Het criterium voor log K_{ow} is 5. Echter, uit de REACH guidance (Appendix R.11-1 Annex 1) blijkt dat stoffen binnen het log K_{ow} gebied van 4 tot 9, bepaald met ClogP, een BCF van 5000 of hoger kunnen hebben.

KoaWin v1.10
Doel: Dit programma berekent de octanol-lucht coëfficiënt (K_{oa}).
Van belang voor: voor bioaccumulatie anders dan in het aquatische milieu.
Criterium: 'Other evidence'. log K_{oa} > 5 met log K_{ow} > 2 in een aanstaande publicatie van Gobas et al.
Prioritering: Hoe hoger de log K_{oa}, hoe hoger de prioritering.
Aantekening: Het programma geeft een schatting op basis van de log K_{ow} en de Henry coëfficiënt. Bij een log K_{ow} < 2 is de uitscheiding via urine zo hoog dat bioaccumulatie ook niet te verwachten is.

Bcfbaf v3.00
Doel: Dit programma berekent de bioaccumulatiefactoren op basis van log K_{ow}, geschat metabolisme (kM) en trofische accumulatie.
Van belang voor: voor bioaccumulatie.
Criterium: BCF >5000
Prioritering: Hoe hoger de BCF, hoe hoger de prioritering; hoe lager de kM, hoe hoger de prioritering

Aantekening: Het programma geeft een schatting op basis van de van de BCF op basis van de hydrofobiteit en van de BAF. In de laatste wordt ook de metabolisme snelheid verwerkt. Echter, de aannames in de berekening zijn onduidelijk. Uit de beschrijving van Bcfbaf wordt ook niet duidelijk over er na de correctie voor metabolisme dubbel gecorrigeerd wordt (de data zijn waarschijnlijk meegenomen in de regressie, die vervolgens een lijn oplevert met een lage richtingscoëfficiënt t.o.v. de QSAR uit de TGD, waarna op de regressie een correctie voor metabolisme wordt toegepast). Het model is nog niet voldoende geanalyseerd om te gebruiken. De mogelijkheid tot accumulatie kan daarom beter worden geschat uit de log K_{ow} waarbij de kM als tweede lijn dient om aan te tonen dat bioaccumulatie waarschijnlijk gering is.

Overig

Wskowwin v1.41 en Waternt v1.01
Doel: Deze programma's berekenen de wateroplosbaarheid.
Van belang voor: indirect de potentie tot bioaccumulatie.
Criterium: geen.
Prioritering: Algemeen hoe lager de wateroplosbaarheid, hoe hoger de prioritering.
Aantekening: Er bestaan verbanden tussen log K_{ow} en de wateroplosbaarheid. De log K_{ow} wordt echter al met twee verschillende programma's geschat. De oplosbaarheid is ook van belang voor het berekenen van de Henry coëfficiënt en daarmee log K_{oa}, maar deze parameters worden ook rechtstreeks geschat.

Henrywin v3.20
Doel: Dit programma berekent de Henry coëfficiënt.
Van belang voor: indirect om de hoeveelheid van een stof gebonden aan aerosolen te bepalen en indirect om de octanol-lucht coëfficiënt (K_{oa}) te bepalen, die van belang is voor bioaccumulatie anders dan in het aquatische milieu.
Criterium: geen.
Prioritering: Geen prioritering.
Aantekening: Het programma geeft zowel een bond als een group methode schatting.

Ecosar v1.00
Niet bekeken vanwege het ontbreken van harde criteria voor toxiciteit, het feit dat het model geen eenduidige resultaten geeft en de kwaliteit van het model nog steeds sterk ter discussie staat.

Appendix 3: Results from the ranking exercise

Selection of substances

Before the final PBT/POP screening assessment was performed by the methodology described in this report, a first screening and ranking assessment was carried out, in which a pre-selection of substances was made before they were ranked. This first exercise was helpful for getting a feeling for the substances, their physical-chemical properties and the ranking criteria, and it still gives a good indication of the numbers of substances fulfilling specific criteria. Therefore, it was considered useful to give a description of this approach and its outcomes here.

A stepwise approach was followed to obtain a final selection and priority setting of potential POP/PBT substances from the total chemical data set. This approach consisted of three different steps, of which the first two were designed to reduce the total set of substances to a subset of those substances that may be harmful with regard to their PBT and POP characteristics. The third step was a step of scoring and ranking in order to make a priority setting within the subset of potential POP/PBT substances. For each of the three steps, selection criteria with regard to P, B, T, and/or LRTP were defined, which are slightly different for the PBT substances selection and for the POP substances selection. This implies that the procedure was to be performed twice, one according to REACH PBT (and vPvB) guidelines and one according to the POP selection procedures in both the Stockholm Convention and the UNECE POP Protocol.

The three-step approach can be described as follows:

1) *Formal screening*
   Selection of substances by strictly following the firm criteria in the REACH protocol or the UNECE-POP Protocol /Stockholm Convention.
2) *Additional 'smart' screening*
   Selection of additional substances that are questionable, but that are kept out of range conform the formal screening criteria.
3) *Scoring and ranking*
   For the different selection criteria parameters, all substances were given a score between 0 and 1 according to their parameter values, and the scores of the individual criteria were summed. Based on the total score, substances were ranked from high to low.

Step 1: formal screening of substances

The first formal screening to select substances was performed based on the screening criteria given either in the Stockholm Convention and the LRTAP Convention for POPs, or in the REACH guidelines for PBT and vPvB substances, as described in section 2.4.1 above.

Within REACH, formal screening criteria only exist for bioaccumulation (B) and persistence (P). As an indicator for P, two different selection criteria were applied, which were regarded as complementary criteria. Following the guidelines, a combination of the outcomes of BioWin3 and BioWin6 or the outcomes of BioWin2 were to be applied to assess biodegradation potential. Within BioWin2, a predicted biodegradability potential of < 0.5 was used as the criterion for potentially high

persistence. 31515 Substances out of the 69152 for which a chemical structure was known fulfilled this criterion. The second criterion indicating potential high persistence (P) was defined as the combination of a biodegradability potential predicted by BioWin6 being < 0.5 and a BioWin3 prediction being < 2.2. In total, 15832 substances fulfilled this criterion, of which 1648 substances were not defined as 'P-substance' according to the former criterion. The 33163 substances that were selected as 'P' following this strategy were taken into account in the assessment of 'B-substances'.
The value of the octanol-water partition coefficient (K_{ow}) was chosen as the indicator for B, with substances being bioaccumulative if they have a log K_{ow} greater than or equal to 4.5. K_{ow}-values of the substances were obtained from KowWin (US-EPA, 2009). By limiting the B assessment to those substances that fulfilled the P criterion, only those substances were selected as potential PBT substance that complied with both the criteria for P and for B. According to this, 8201 substances were finally selected in the formal screening step for PBTs.

Within both POP conventions, the criterion for P to be a potential POP is an aquatic half-life of more than 60 days. These half-lives were derived from a combination of Biowin3 outcomes and a conversion method described by Aronson et al. (2006). The bioaccumulation criterion in both POP conventions is given by a bioaccumulation factor (BCF) of more than 5000, derived by BCFwin (US-EPA, 2009). Similar to the REACH PBT guidelines, substances were selected as potential POPs only when they fulfilled both the criteria with respect to P and B. 1131 Substances out of the 69152 for which structure information was available were selected.

Step 2: additional 'smart' screening of substances
In addition to the formal screening, a more advanced screening was performed to select additional substances that are questionable, so that they might be POP/PBT substances, but are kept out of range conform to the formal screening criteria. For the PBT assessment, this 'smart' screening includes: B: the addition of substances that have an octanol-air partition coefficient (K_{oa}) larger than 6, in combination with a vapour pressure > 100 Pa and an atmospheric half-life > 48 hours (conform AopWin; US-EPA, 2009), even if log K_{ow} is smaller than 4.5. This was done conform to Gobas et al. (2006), who proved the bioaccumulation potential via air of substances having a K_{oa} that is so high. P: beside the biodegradation potential as an indicator for persistence, the half-life of a substance in water was taken as an additional indicator. Substances with a half-life greater than or equal to 40 days were added to the selection.
For the PBT assessment, the 'smart' screening resulted in the addition of 1758 substances to the list of substances derived from the formal screening, of which 1727 substances were selected based on the additional P-criterion, and 31 based on the additional B-criterion. Consequently, the final list of substances from the formal and smart screening together contained 9959 substances.

Within the Stockholm Convention and UNECE POP protocol, except for P and B, quantitative criteria exist for the selection of substances according to their long-range transport potential (LRTP). For the POP assessment, in the 'smart' screening step, the half-life in air was added as a criterion for substances to be a potential POP. Following the conventions, LRTP was assessed based on the half-life of a substance in the air, which has to be larger than 2. The atmospheric half-life of the substances was derived from AopWin (US-EPA, 2009). The inclusion of this LRTP criterion resulted in the addition of 40 substances to the POP-screening list, resulting in a final screening list of 1171 substances.

An overview of the criteria and data sources of the formal screening and additional 'smart' screening steps for PBT and POP selection are presented in the upper part of Table 1. The screening steps are also presented schematically in Figure 1 for the PBT-assessment and in Figure 2 for the POP-assessment.

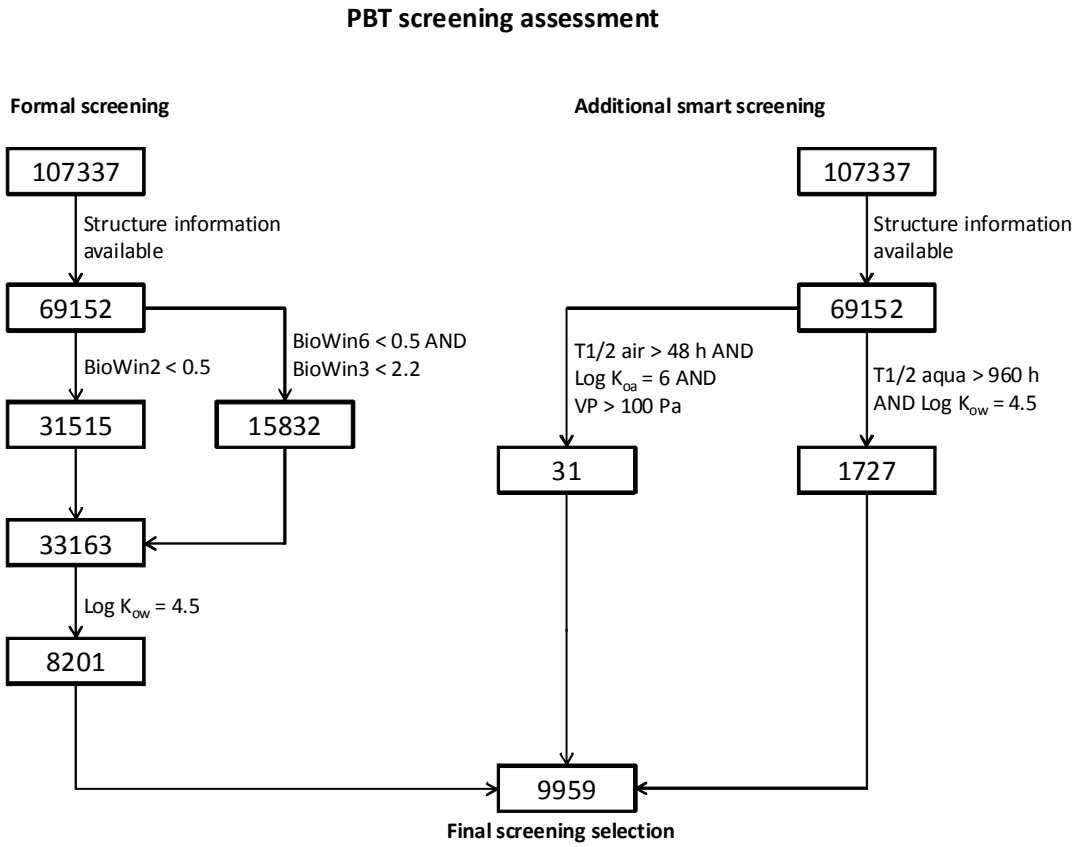

Figure 1. Schematic overview of the screening steps incorporated in the formal screening and smart screening of the PBT assessment. The numbers in the boxes indicate the number of substances fulfilling the described criteria.

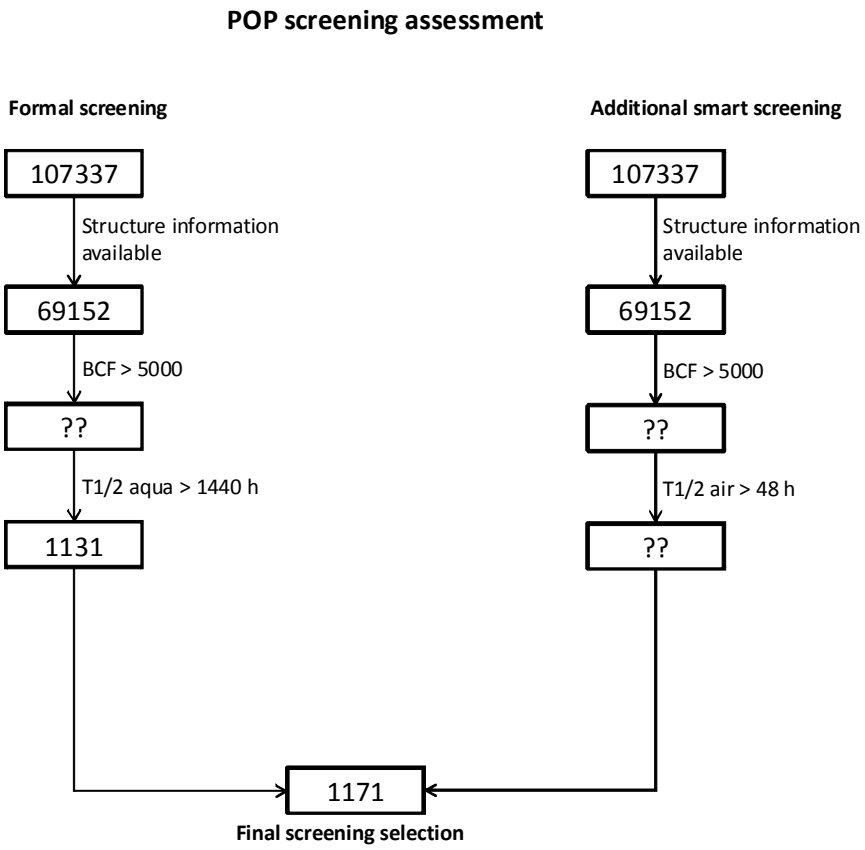

Figure 2. Schematic overview of the screening steps incorporated in the formal screening and smart screening of the POP assessment. The numbers in the boxes indicate the number of substances fulfilling the described criteria.

Step 3: sorting and ranking of the substances

After the two selections of substances were made out of the total set of 69152 chemical substances according to the formal and smart screening criteria for PBT and POP, those substances that were considered most similar to the POP/PBT-substance descriptions were to be selected. This priority setting of substances was performed by a 'sorting and ranking' step. In this step, for both the PBT assessment and the POP assessment, a more advanced assessment of P, B was performed, similar to the assessments described in this report, which could not be handled for the total set of substances but could for the subset. In addition, for the POP assessment solely, an assessment of the LRTP of the substances was made and taken into account in the ranking procedure. An overview of the assessment strategy of P, B and LRTP is listed in Table 1.

#	Step:	REACH (PBT/vPvB)		POP (UNEP	
		Criterion	**Data source**	**Criterion**	**Data source**
1	**'Rigid' screening**	**P:** biodeg < 0.5 **B:** log K_{ow} ≥ 4.5	**P:** BioWin2+3[1] or BioWin2+6[1] **B:** KowWin[1]	**P:** T1/2 aqua > 60 d **B:** BCF > 5000	**P:** BioWin3[1], Aronson et al., 2006 **B:** BCFWin[1]
2	**Additional 'smart' screening**	**P:** T1/2 aqua > 40 d **B:** log K_{oa} > 6 (even if log K_{ow} < 4.5) **LRTP:** T1/2 air > 2 d	**P:** Aronson et al. **B:** Gobas et al., 200x **LRTP:** AopWin[1]	**LRTP:** T1/2 air > 2 d	**LRTP:** AopWin[1]
3	**Scoring + ranking**	**P:** P_{ov} **B:** See main text of report	**P:** OECD tool (linear scaling) **B:** See main text of report	**P:** P_{ov} **B:** See main text of report **LRTP:** CTD	**P:** OECD tool (linear scaling) **B:** See main text of report **LRTP:** OECD tool (linear scaling)

[1] EpiSuite software, US-EPA

Table 1: Overview of the criteria and data sources of the formal screening and additional 'smart' screening steps for PBT and POP selection, and the procedures followed for sorting and ranking of selected substances.

Results of the ranking procedure

Top 10 based on:

B-ranking *(with B=0.4*B(log K_{ow}) + 0.3*B(log K_{oa}) + 0.3*B(kM))*

rank	MW	MolForm	Name	CAS nr.
10	523.97	C28H27ClF5NO	Penfluridol	26864-56-2
9	445.04	C26H37ClN2O2	EINECS 257-219-1	51461-11-1
8	669.84	C36H43N7O4S	EINECS 275-044-9	70942-39-1
7	641.70	C12H18Br6	HBCDD (hexabromo cyclododecane)	25637-99-4
6	314.46	C24H26	4-(1,3-Diphenylbutyl)-m-xylene	84255-43-6
5	314.46	C24H26	2-(1,3-diphenylbutyl)-1,3-dimethylbenzene	94279-12-6
4	314.46	C24H26	4-(1,3-diphenylbutyl)-1,2-dimethylbenzene	56525-86-1
3	314.46	C24H26	1-(2,4-diphenylpentyl)-2-methylbenzene	74921-47-4
2	314.46	C24H26	2-(1,3-Diphenylbutyl)-p-xylene	84255-44-7
1	372.55	C26H32N2	N,N'-Bis(4-(tert-butyl)phenyl)benzene-1,4-diamine	5432-99-5

P-ranking

rank	MW	MolForm	Name	CAS nr.
10	448.95	C7BrF15	Perfluoroheptyl bromide	375-88-2
9	354.50	C6ClF13	Perfluorohexyl chloride	355-41-9
8	521.07	C9F21N	Perfluamine	338-83-0
7	388.05	C7F16	Perfluoroheptane	335-57-9
6	516.07	C10F20O	EINECS 274-065-0	69661-30-9
5	462.08	C10F18	Perflunafene	306-94-5
4	500.08	C10F20	Perfluoro-n-butylcyclohexane	374-60-7
3	566.08	C11F22O	Octadecafluoro-9-(trifluoromethyl)decanoyl fluoride	15720-98-6
2	438.06	C8F18	1,1,1,2,2,3,4,5,5,6,6,6-dodecafluoro-3,4-bis(trifluoromethyl)hexane	1735-48-4
1	488.06	C9F20	1,1,1,2,2,3,4,5,5,5-Decafluoro-3-(1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl)-4-(trifluoromethyl)pentane	50285-18-2

LRTranking

rank	MW	MolForm	Name	CAS nr.
10	495.96	C7F15I	Perfluoroheptyl iodide	335-58-0
9	398.95	C6BrF13	Perfluorohexyl bromide	335-56-8
8	448.95	C7BrF15	Perfluoroheptyl bromide	375-88-2
7	354.50	C6ClF13	Perfluorohexyl chloride	355-41-9
6	388.05	C7F16	Perfluoroheptane	335-57-9
5	462.08	C10F18	Perflunafene	306-94-5
4	500.08	C10F20	Perfluoro-n-butylcyclohexane	374-60-7
3	566.08	C11F22O	Octadecafluoro-9-(trifluoromethyl)decanoyl fluoride	15720-98-6
2	438.06	C8F18	1,1,1,2,2,3,4,5,5,6,6,6-Dodecafluoro-3,4-bis(trifluoromethyl)hexane	1735-48-4
1	488.06	C9F20	1,1,1,2,2,3,4,5,5,5-Decafluoro-3-(1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl)-4-(trifluoromethyl)pentane	50285-18-2

Appendix 4. 250 substances with the highest PB-scores

Substances which have been discussed in the Results section have their names indicated in **boldface.**

Rank	CAS RN	Name	MW	Ctgb	Alanwood	Biocide	EINECS	INN	PAN	EPA	P-score	B-score	PB-score
1	93819-97-7	N,N-Bis(2-hydroxyethyl)-4-((4,4,5,5,5-pentafluoro-3-(pentafluoroethyl)-1,2,3-tris(trifluoromethyl)pent-1-enyl)oxy)benze	741.4				x				**1.00**	**0.99**	**1.99**
2	2385-85-5	**Mirex**	545.5		x		x		x		**1.00**	**0.98**	**1.98**
3	39765-80-5	TRANS-NONACHLOR	444.2						x		**0.99**	**0.99**	**1.98**
4	10386-84-2	4,4'-Dibromooctafluorobiphenyl	455.9				x				**1.00**	**0.98**	**1.98**
5	5566-34-7	**GAMMA-CHLORDANE**	409.8				x				**0.99**	**0.98**	**1.98**
6	18291-67-3	Silane, dichloro(1,4,5,6,7,7-hexachloro-5-norbornen-2-yl)methyl-	413.8				x				**0.99**	**0.98**	**1.97**
7	2550-75-6	Chlorbicyclen, HERCULES426	397.8		x				x		**0.99**	**0.99**	**1.97**
8	57-74-9	**Chlordane**	409.8		x		x				**0.99**	**0.98**	**1.97**
9	5103-71-9	**cis-Chlordane (alpha-)**	409.8				x				**0.99**	**0.98**	**1.97**
10	5103-74-2	**trans-Chlordane**	409.8				x				**0.99**	**0.98**	**1.97**
11	93894-52-1	1,1,2,3,3,3-Hexafluoro-2-(trifluoromethyl)propane-1-sulphonic anhydride	582.2				x				**1.00**	**0.97**	**1.97**
12	70281-93-5	Potassium N-((heptadecafluorooctyl)sulphonyl)-N-methylglycinate	570.2				x				**0.98**	**0.98**	**1.97**
13	97298-47-0	perfluorinated octanoic acid (PFOA) derivative	571.2				x				**0.98**	**0.98**	**1.97**
14	24448-09-7	1-Octanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-N-(2-hydroxyethyl)-N-methyl-	557.2				x				**0.99**	**0.98**	**1.97**
15	1691-99-2	1-Octanesulfonamide, N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-N-(2-hydroxyethyl)-	571.3				x				**0.99**	**0.97**	**1.96**
16	68239-75-8	1-Heptanesulfonamide, N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-N-[3-(trimethoxysilyl)propyl]-	639.5				x				**0.98**	**0.98**	**1.96**
17	8001-35-2	**Toxaphene**	413.8		x		x		x		**0.99**	**0.97**	**1.96**
18	78974-42-2	perfluorinated octanoic acid (PFOA) derivative	593.1				x				**1.00**	**0.96**	**1.96**
19	18106-12-2	2-Norbornene, 1,2,3,4,7,7-hexachloro-5-(diethoxymethylsilyl)-	433.1				x				**0.98**	**0.98**	**1.96**
20	67584-62-7	Glycine, N-ethyl-N-[(pentadecafluoroheptyl)sulfonyl]-, potassium salt	534.2				x				**0.98**	**0.98**	**1.96**
21	68957-63-1	Glycine, N-ethyl-N- (pentadecafluoroheptyl)sulfonyl -	535.2				x				**0.98**	**0.98**	**1.96**
22	25935-14-2	perfluorinated octanoic acid (PFOA) derivative	526.2				x				**0.97**	**0.99**	**1.96**
23	2991-50-6	Glycine, N-ethyl-N- (heptadecafluorooctyl)sulfonyl -	584.2				x				**0.99**	**0.97**	**1.96**
24	68298-89-5	1-Heptanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-N-(4-hydroxybutyl)-N-methyl-	535.3				x				**0.99**	**0.97**	**1.96**
25	18300-04-4	dibromo-Chlordene	498.7				x				**0.98**	**0.97**	**1.96**
26	68412-68-0	Phosphonic acid, perfluoro-C6-12-alkyl derivs.	500.0	x			x				**0.99**	**0.96**	**1.96**
27	13252-14-7	perfluorinated octanoic acid (PFOA) derivative	495.1				x				**0.98**	**0.98**	**1.96**
28	309-00-2	**Aldrin**	364.9		x		x		x		**0.97**	**0.98**	**1.96**
29	465-73-6	**Aldrin**	364.9		x		x		x		**0.97**	**0.98**	**1.96**
30	68555-67-9	1-Octanesulfinic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-, sodium salt	483.1				x				**0.99**	**0.97**	**1.95**
31	68631-02-7	**tetrachloro-DDT**	388.9				x				**0.97**	**0.98**	**1.95**
32	68555-73-7	1-Heptanesulfonamide, N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-N-(2-hydroxyethyl)-	521.2				x				**0.98**	**0.97**	**1.95**
33	29082-74-4	Octachlorostyrene	379.7						x		**0.97**	**0.98**	**1.95**
34	2051-24-3	**Decachlorobiphenyl**	498.7				x				**0.99**	**0.96**	**1.95**

Rank	CAS RN	Name	MW	Ctgb	Alanwood	Biocide	EINECS	INN	PAN	EPA	P-score	B-score	PB-score
35	14168-01-5	BETA-DIHYDROHEPTACHLOR	375.3		x						**0.97**	**0.98**	**1.95**
36	76-44-8	**Heptachlor**	373.3		x		x		x		**0.97**	**0.98**	**1.95**
37	61660-12-6	1-Octanesulfonamide, N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-N-[3-(trimethoxysilyl)propyl]-	689.5				x				**0.98**	**0.96**	**1.94**
38	4089-58-1	Propanoyl fluoride, 2,3,3,3-tetrafluoro-2-(1,1,2,3,3,3-hexafluoro-2-(1,1,2,2-tetrafluoro-2-(fluorosulfonyl)ethoxy)propoxy	512.1				x				**0.99**	**0.95**	**1.94**
39	68310-02-1	1-Heptanesulfonamide, N-butyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-N-(2-hydroxyethyl)-	549.3				x				**0.98**	**0.97**	**1.94**
40	18052-83-0	Silane, triethoxy(1,4,5,6,7,7-hexachlorobicyclo[2.2.1]hept-5-en-2-yl)-	463.1				x				**0.98**	**0.96**	**1.94**
41	1043-50-1	Decafluorodiphenyl sulfide	366.2				x				**0.99**	**0.95**	**1.94**
42	68555-76-0	1-Heptanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-N-(2-hydroxyethyl)-N-methyl-	507.2				x				**0.98**	**0.96**	**1.94**
43	85284-15-7	Sodium 4-((1,3,4,5,5,5-hexafluoro-1-(pentafluoroethyl)-2,4-bis(trifluoromethyl)-2-pentenyl)oxy)benzenesulphonate	603.2				x				**0.97**	**0.97**	**1.94**
44	68239-73-6	1-Octanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-N-(4-hydroxybutyl)-N-methyl-	585.3				x				**0.99**	**0.95**	**1.94**
45	51936-55-1	1,4-Methanobenzocyclooctene, 7,8-dibromo-1,2,3,4,11,11-hexachloro-1,4,4a,5,6,7,8,9,10,10a-decahydro-	540.8				x				**0.99**	**0.95**	**1.94**
46	40630-61-3	Heptadecafluoro-N,N-bis(2-hydroxyethyl)octanesulphonamide	587.3				x				**0.99**	**0.95**	**1.94**
47	72-20-8	**Endrin**	380.9		x		x		x		**0.97**	**0.97**	**1.94**
48	60-57-1	**Dieldrin**	380.9		x		x	x	x		**0.97**	**0.97**	**1.94**
49	85665-66-3	potassium N-propyl-N-[(tridecafluorohexyl)sulphonyl]glycinate	498.2				x				**0.96**	**0.98**	**1.94**
50	93857-44-4	Diammonium 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl phosphate	543.1				x				**0.99**	**0.94**	**1.94**
51	475-26-3	**DFDT**	321.6				x		x		**0.96**	**0.97**	**1.94**
52	13417-01-1	1-Octanesulfonamide, N- 3-(dimethylamino)propyl -1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-	584.3				x				**0.99**	**0.94**	**1.94**
53	1715-40-8	**Bromocyclene**	393.7		x		x	x	x		**0.97**	**0.97**	**1.93**
54	52584-45-9	sodium 4-[1,1,1,5,5,6,6,6-octafluoro-4-(1,1,2,2,2-pentafluoroethyl)-3,4-bis(trifluoromethyl)hex-2-en-2-yl]oxybenzenesulf	653.2				x				**0.95**	**0.99**	**1.93**
55	70729-63-4	N,N-dibutylbutan-1-amine; 4-[(E)-1,1,1,5,5,6,6,6-octafluoro-4-(1,1,2,2,2-pentafluoroethyl)-3,4-bis(trifluoromethyl)hex-2	653.2				x				**0.95**	**0.99**	**1.93**
56	17202-41-4	1-Nonanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-nonadecafluoro-, ammonium salt	549.1				x				**0.96**	**0.97**	**1.93**
57	18134-58-2	Silane, trichloro(1,4,5,6,7,7-hexachloro-5-norbornen-2-yl)-	434.3				x				**0.98**	**0.95**	**1.93**
58	1506-15-6	1,2,3,4,5,6-Hexachloro-7-methoxynaphthalene	364.9				x				**0.95**	**0.98**	**1.93**
59	94042-94-1	Sodium 4-((1,4,4,5,5,5-hexafluoro-1,2,3-tris(trifluoromethyl)-2-pentenyl)oxy)benzenesulphonate	553.2				x				**0.97**	**0.95**	**1.93**
60	67584-54-7	1-Heptanesulfonamide, N- 3-(dimethylamino)propyl -1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-	534.3				x				**0.99**	**0.94**	**1.93**
61	754-91-6	Perfluoroctylsulfonamide	499.1				x				**1.00**	**0.93**	**1.93**
62	67584-53-6	Glycine, N-ethyl-N-[(tridecafluorohexyl)sulfonyl]-, potassium salt	484.2				x				**0.96**	**0.97**	**1.93**
63	68957-32-4	Glycine, N-ethyl-N- (tridecafluorohexyl)sulfonyl -	485.2				x				**0.96**	**0.97**	**1.93**
64	67939-96-2	2-Propenoic acid, 2-methyl-, 2- methyl (pentadecafluoroheptyl)sulfonyl amino ethyl ester	575.3				x				**0.99**	**0.94**	**1.93**
65	68084-62-8	2-Propenoic acid, 2- methyl (pentadecafluoroheptyl)sulfonyl amino ethyl ester	561.3				x				**0.98**	**0.94**	**1.93**
66	93894-55-4	1,1,2,2,3,3,4,4-Octafluorobutane-1-sulphonic anhydride	546.2				x				**0.98**	**0.95**	**1.93**
67	55591-23-6	1,1,2,2,3,3,4,4,5,5,6,6,6-Tridecafluorohexane-1-sulphonyl chloride	418.6				x				**1.00**	**0.93**	**1.92**
68	66008-69-3	2-Propenoic acid, 2- (2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-heptadecafluorononyl)sulfonyl methylamino ethyl ester	625.3				x				**0.97**	**0.95**	**1.92**
69	94042-95-2	Sodium 4-((1,3,4,4,5,5,5-heptafluoro-2-(2,2,3,3,3-pentafluoro-1-(pentafluoroethyl)-1-(trifluoromethyl)propyl)-3-(trifluor	753.3				x				**0.94**	**0.98**	**1.92**
70	94158-62-0	1-(2-(2-Butoxyethoxy)ethoxy)-4,4,5,5,6,6,7,7,8,8,9,9,10,11,11,11-hexadecafluoro-10-(trifluoromethyl)undecan-2-ol	688.4				x				**1.00**	**0.93**	**1.92**
71	423-50-7	1-Hexanesulfonyl fluoride, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-	402.1				x				**1.00**	**0.92**	**1.92**
72	28680-45-7	Bicyclo[2.2.1]hept-2-ene, heptachloro-	335.3				x				**0.96**	**0.97**	**1.92**
73	59071-10-2	2-Propenoic acid, 2- ethyl (pentadecafluoroheptyl)sulfonyl amino ethyl ester	575.3				x				**0.99**	**0.94**	**1.92**

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74	68239-74-7	1-Hexanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-N-(4-hydroxybutyl)-N-methyl-	485.3				x				**0.97**	**0.95**	**1.92**
75	94158-61-9	1-(2-(2-Butoxyethoxy)ethoxy)-4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-heptadecafluoroundecan-2-ol	638.4				x				**0.99**	**0.93**	**1.92**
76	881-99-2	alpha,alpha'-Hexachloro-m-xylene	312.8				x				**0.95**	**0.97**	**1.92**
77	67906-70-1	2-Propenoic acid, 2-methyl-, 2- ethyl (tridecafluorohexyl)sulfonyl amino ethyl ester	539.3				x				**0.98**	**0.94**	**1.92**
78	55910-10-6	N-Propyl-N-((heptadecafluorooctyl)sulfonyl)glycine, potassium salt	598.3				x				**0.99**	**0.93**	**1.92**
79	24407-09-8	[4,4,5,5,6,6,7,7,8,8,9,9,10,11,11,11-hexadecafluoro-2-hydroxy-10-(trifluoromethyl)undecyl] prop-2-enoate	598.2				x				**0.98**	**0.94**	**1.92**
80	789-02-6	**o,p'-DDT**	354.5				x				**0.94**	**0.98**	**1.92**
81	33979-03-2	**2,2',4,4',6,6'-PCB**	360.9				x				**0.93**	**0.98**	**1.92**
82	50-29-3	**DDT**	354.5		x	x	x	x			**0.94**	**0.98**	**1.92**
83	335-77-3	1-Decanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heneicosafluoro-	599.1				x				**0.97**	**0.95**	**1.92**
84	434-90-2	Decafluorobiphenyl	334.1				x				**0.96**	**0.96**	**1.92**
85	2888-15-5	1,1'-Methylenebis(2,4,5-trichlorobenzene)	374.9				x				**0.95**	**0.97**	**1.92**
86	16090-14-5	Ethanesulfonyl fluoride, 2- 1- difluoro (trifluoroethenyl)oxy methyl -1,2,2,2-tetrafluoroethoxy -1,1,2,2-tetrafluoro-	446.1				x				**0.95**	**0.97**	**1.92**
87	7421-93-4	**ENDRIN ALDEHYDE**	380.9						x		**0.98**	**0.94**	**1.91**
88	81613-60-7	Piperidine, 1-(3-(3,5-bis(trifluoromethyl)phenyl)-2-propynyl)-4-(1,1-dimethylethyl)-, hydrochloride	391.4				x				**0.97**	**0.95**	**1.91**
89	42115-16-2	Pentachloro(2,3-dibromopropoxy)benzene	466.2				x				**0.94**	**0.97**	**1.91**
90	1335-87-1	**Naphthalene, hexachloro-**	334.8				x				**0.93**	**0.98**	**1.91**
91	1024-57-3	**Heptachlor epoxide**	389.3				x		x		**0.97**	**0.94**	**1.91**
92	67939-61-1	2-Propenoic acid, 2-methyl-, 4- methyl (tridecafluorohexyl)sulfonyl amino butyl ester	553.3				x				**0.98**	**0.93**	**1.91**
93	59493-82-2	p-((Undecafluorohexenyl)oxy)benzenesulphonyl chloride	472.7				x				**0.93**	**0.98**	**1.91**
94	67584-61-6	2-Propenoic acid, 2-methyl-, 2- methyl (tridecafluorohexyl)sulfonyl amino ethyl ester	525.3				x				**0.97**	**0.93**	**1.91**
95	50285-18-2	1,1,1,2,2,3,4,5,5,5-Decafluoro-3-(1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl)-4-(trifluoromethyl)pentane	488.1				x				**1.00**	**0.91**	**1.91**
96	4236-15-1	Heptadecafluoro-N-(2-hydroxyethyl)-N-propyloctanesulphonamide	585.3				x				**0.99**	**0.92**	**1.91**
97	68227-98-5	4-(Methyl((tridecafluorohexyl)sulphonyl)amino)butyl acrylate	539.3				x				**0.98**	**0.93**	**1.91**
98	67525-36-4	1,4-Bis(4-(trifluoromethyl)phenoxy)benzene	398.3				x				**0.94**	**0.97**	**1.91**
99	1107-00-2	1,3-Isobenzofurandione, 5,5'- 2,2,2-trifluoro-1-(trifluoromethyl)ethylidene bis-	444.2				x				**0.96**	**0.95**	**1.90**
100	65294-20-4	Benzene, 1,1'- 2,2,2-trifluoro-1-(trifluoromethyl)ethylidene bis 3,4-dimethyl-	360.3				x				**0.94**	**0.97**	**1.90**
101	1782-06-5	Chloran	424.9				x				**0.98**	**0.92**	**1.90**
102	34455-03-3	1-Hexanesulfonamide, N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-N-(2-hydroxyethyl)-	471.2				x				**0.97**	**0.93**	**1.90**
103	85665-64-1	Tridecafluoro-N-(2-hydroxyethyl)-N-propylhexanesulphonamide	485.3				x				**0.97**	**0.93**	**1.90**
104	2227-17-0	Dienochlor	474.6	x	x		x		x		**0.99**	**0.91**	**1.90**
105	2234-13-1	**Naphthalene, octachloro-**	403.7				x				**0.98**	**0.92**	**1.90**
106	28031-44-9	2,2'-((2,2',3,3',5,5',6,6'-Octachloro(1,1'-biphenyl)-4,4'-diyl)bis(oxyethane-2,1-diyloxy))bisethanol	638.0				x				**0.99**	**0.91**	**1.90**
107	32241-08-0	**Naphthalene, heptachloro-**	369.3				x				**0.96**	**0.94**	**1.90**
108	68555-66-8	1-Heptanesulfinic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-, sodium salt	433.1				x				**0.98**	**0.92**	**1.90**
109	115-32-2	**Dicofol**	370.5	x	x	x	x		x	x	**0.95**	**0.94**	**1.89**
110	1735-48-4	1,1,1,2,2,3,4,5,5,6,6,6-Dodecafluoro-3,4-bis(trifluoromethyl)hexane	438.1				x				**1.00**	**0.89**	**1.89**
111	16557-94-1	Ammonium 8-chlorotetradecafluorooctanoate	429.5				x				**0.92**	**0.97**	**1.89**
112	68318-36-5	1-Propanaminium, 3- (carboxymethyl) (heptadecafluorooctyl)sulfonyl amino -N,N,N-trimethyl-, hydroxide, inner salt	656.4				x				**0.99**	**0.90**	**1.89**

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113	25268-77-3	2-Propenoic acid, 2- (heptadecafluorooctyl)sulfonyl methylamino ethyl ester	611.3				x				**0.99**	**0.90**	**1.89**
114	69013-34-9	Benzenesulfonamide, N-methyl-4- 4,4,5,5,5-pentafluoro-3-(pentafluoroethyl)-1,2,3-tris(trifluoromethyl)-1-pentenyl oxy	790.3				x				**1.00**	**0.89**	**1.89**
115	1893-52-3	Propenoic acid, 2- ethyl (tridecafluorohexyl)sulfonyl amino ethyl ester	525.3				x				**0.97**	**0.91**	**1.89**
116	1763-23-1	1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-	499.1				x				**0.94**	**0.95**	**1.89**
117	3734-48-3	**Chlordene (isomer mixture)**	338.9				x				**0.94**	**0.95**	**1.89**
118	25429-29-2	**PENTACHLOROBIPHENYL**	326.4				x				**0.90**	**0.99**	**1.89**
119	3658-57-9	Ammonium 8-chlorohexadecafluoro-7-methyloctanoate	479.5				x				**0.91**	**0.98**	**1.89**
120	83721-47-5	Methanesulfonamide, 1-chloro-N-[2,3,4-trichloro-6-(2,4-dichlorophenoxy)phenyl]-, sodium salt	492.0				x				**0.96**	**0.92**	**1.89**
121	94248-26-7	Methanesulfonamide, 1-chloro-N-(2-phenoxyphenyl)-, pentachloro deriv., sodium salt	492.0				x				**0.96**	**0.92**	**1.89**
122	55485-74-0	Flophemesyldiethylamine	297.3				x				**0.97**	**0.92**	**1.88**
123	68957-54-0	Glycine, N-ethyl-N- (pentadecafluoroheptyl)sulfonyl -, ethyl ester	563.3				x				**0.95**	**0.93**	**1.88**
124	3883-86-1	1,1'-Biphenyl, 2,2',3,3',5,5',6,6'-octafluoro-	298.1				x				**0.94**	**0.94**	**1.88**
125	56860-12-9	3-(2,2-Dichlorovinyl)-2,2-dimethylcyclopropanecarboxylic anhydride	400.1				x				**0.93**	**0.95**	**1.88**
126	53494-70-5	**ENDRIN KETONE**	380.9						x		**0.98**	**0.90**	**1.88**
127	85118-22-5	2-bromo-1-[chloro-(4-fluorophenyl)methyl]-4-(trifluoromethyl)benzene	367.6				x				**0.92**	**0.96**	**1.88**
128	68227-97-4	4-[methyl(1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoroheptylsulfonyl)amino]butyl prop-2-enoate	589.3				x				**0.99**	**0.89**	**1.88**
129	34598-33-9	4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-heptadecafluoroundecanoic acid	491.1				x				**0.94**	**0.94**	**1.88**
130	42115-15-1	(Allyloxy)pentachlorobenzene	306.4				x				**0.89**	**0.98**	**1.88**
131	67906-40-5	2-Propenoic acid, 2-methyl-, 4- methyl (undecafluoropentyl)sulfonyl amino butyl ester	503.3				x				**0.96**	**0.91**	**1.88**
132	34482-99-0	**Fletazepam**	356.7				x	x			**0.95**	**0.93**	**1.88**
133	69661-30-9	2,3,5-trifluoro-4-(1,1,2,2,2-pentafluoroethyl)-2,3,4,5-tetrakis(trifluoromethyl)oxolane	516.1				x				**1.00**	**0.87**	**1.87**
134	67939-36-0	2-Propenoic acid, 2-methyl-, 2- ethyl (pentadecafluoroheptyl)sulfonyl amino ethyl ester	589.3				x				**0.99**	**0.88**	**1.87**
135	62601-17-6	1,2,3,4,5-pentachloro-6-(chloromethylsulfanyl)benzene	330.9				x				**0.93**	**0.95**	**1.87**
136	297-78-9	Isobenzan	411.8		x		x		x		**0.99**	**0.88**	**1.87**
137	73353-25-0	2-carboxyethyl-[3-[[4,4,5,5,6,6,7,7,8,8,9,9,10,11,11,11-hexadecafluoro-2-hydroxy-10-	701.4				x				**1.00**	**0.87**	**1.87**
138	68555-75-9	1-Hexanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-N-(2-hydroxyethyl)-N-methyl-	457.2				x				**0.96**	**0.91**	**1.87**
139	1544-19-0	1-(1,1,2,2-tetrafluoroethoxy)-4-[2-[4-(1,1,2,2-tetrafluoroethoxy)phenyl]propan-2-yl]benzene	428.3				x				**0.88**	**0.98**	**1.86**
140	32534-81-9	Benzene, 1,1 -oxybis-, pentabromo deriv.	564.7				x				**0.93**	**0.93**	**1.86**
141	76784-42-4	1-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2,2,2-trichloroethanone	419.5				x				**0.99**	**0.88**	**1.86**
142	94159-85-0	1-(aziridin-1-yl)-4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-heptadecafluoroundecan-2-ol	519.2				x				**0.98**	**0.88**	**1.86**
143	5736-49-2	Decafluorobenzhydryl bromide	427.0				x				**0.98**	**0.88**	**1.86**
144	1652-63-7	1-Propanaminium, 3-[[(heptadecafluorooctyl)sulfonyl]amino]-N,N,N-trimethyl-, iodide	599.3				x				**1.00**	**0.87**	**1.86**
145	53542-48-6	9-(3-chloropropyl)-6-fluoro-2-(trifluoromethyl)-9H-thioxanthene	360.8				x				**0.93**	**0.93**	**1.86**
146	51800-99-8	(1R,4R)-2-(2,2,3,3,4,4,4-heptafluorobutanoyl)-4,7,7-trimethylbicyclo[2.2.1]heptan-3-one	348.3				x				**0.95**	**0.91**	**1.86**
147	94349-23-2	methoxymethyl-bis[(4,7,7-trimethyl-3-bicyclo[2.2.1]heptanyl)oxy]silicon	380.6				x				**0.88**	**0.98**	**1.86**
148	335-57-9	Heptane, hexadecafluoro-	388.0				x				**1.00**	**0.86**	**1.86**
149	26604-52-4	Tris(dichloropropyl) phosphite	414.9				x				**0.98**	**0.88**	**1.86**
150	2172-49-8	3,3,3-tris(4-chlorophenyl)propanoyl chloride	424.1				x				**0.90**	**0.96**	**1.86**
151	94159-86-1	1-ethenoxy-4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-heptadecafluoroundecan-2-ol	520.2				x				**0.90**	**0.96**	**1.86**

Rank	CAS RN	Name	MW	Ctgb	Alanwood	Biocide	EINECS	INN	PAN	EPA	P-score	B-score	PB-score
152	67584-57-0	2-Propenoic acid, 2- methyl (tridecafluorohexyl)sulfonyl amino ethyl ester	511.3				x				**0.97**	**0.89**	**1.86**
153	68298-10-2	1-Heptanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-N-(phenylmethyl)-	539.3				x				**0.98**	**0.88**	**1.86**
154	375-81-5	1-Pentanesulfonyl fluoride, 1,1,2,2,3,3,4,4,5,5,5-undecafluoro-	352.1				x				**1.00**	**0.86**	**1.86**
155	34367-37-8	[4-(trifluoromethoxy)phenyl]-[4-(trifluoromethyl)phenyl]methanone	334.2				x				**0.91**	**0.95**	**1.86**
156	87996-57-4	[4-(trifluoromethoxy)phenyl]-[2-(trifluoromethyl)phenyl]methanone	334.2				x				**0.91**	**0.95**	**1.86**
157	83721-46-4	Methanesulfonamide, 1-chloro-N-[4,5-dichloro-2-(2,4-dichlorophenoxy)phenyl]-, sodium salt	457.5				x				**0.94**	**0.92**	**1.86**
158	127-90-2	1,1'-Oxybis[2,3,3,3-tetrachloropropane]	377.7			x	x		x		**0.98**	**0.87**	**1.86**
159	83929-68-4	1,2,3,4-tetrabromo-5-methyl-6-prop-2-enoxybenzene	463.8				x				**0.89**	**0.97**	**1.85**
160	1321-64-8	**Naphthalene, pentachloro-**	300.4				x				**0.88**	**0.97**	**1.85**
161	67584-49-0	1-Heptanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-N-2-propenyl-	489.2				x				**0.90**	**0.95**	**1.85**
162	76253-60-6	**TETRACHLOROBENZYLTOLUENE**	320.0				x				**0.89**	**0.96**	**1.85**
163	143-50-0	**Chlordecone**	490.6	x	x		x		x		**1.00**	**0.85**	**1.85**
164	36065-30-2	2,4,6-TRIBROMOPHENYL(2-METHYL-2,3-DIBROMOPROPYL)	544.7				x				**0.91**	**0.94**	**1.85**
165	67906-73-4	2-Propenoic acid, 2-methyl-, 2- ethyl (undecafluoropentyl)sulfonyl amino ethyl ester	489.3				x				**0.96**	**0.89**	**1.85**
166	51032-47-4	Sodium 2-[(1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluorooctylsulfonylamino)methyl]benzenesulfonate	668.3				x				**1.00**	**0.85**	**1.85**
167	3389-71-7	Bicyclo 2.2.1 hepta-2,5-diene, 1,2,3,4,7,7-hexachloro-	298.8				x				**0.92**	**0.92**	**1.85**
168	67584-52-5	Glycine, N-ethyl-N-[(undecafluoropentyl)sulfonyl]-, potassium salt	434.2				x				**0.92**	**0.92**	**1.85**
169	68957-31-3	Glycine, N-ethyl-N- (undecafluoropentyl)sulfonyl -	435.2				x				**0.92**	**0.92**	**1.85**
170	118-74-1	**Benzene, hexachloro-**	284.8		x		x		x		**0.92**	**0.93**	**1.85**
171	50598-28-2	1-Hexanesulfonamide, N- 3-(dimethylamino)propyl -1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-	484.3				x				**0.98**	**0.86**	**1.84**
172	85721-09-1	2-Bromo-4'-fluoro-4-(trifluoromethyl)benzophenone	347.1				x				**0.91**	**0.93**	**1.84**
173	94159-76-9	bis(2-hydroxyethyl)-methyl-[4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,15,15,15-tetracosafluoro-2-hydroxy-14-(	846.3				x				**1.00**	**0.84**	**1.84**
174	15720-98-6	Decanoyl fluoride, octadecafluoro-9-(trifluoromethyl)-	566.1				x				**1.00**	**0.84**	**1.84**
175	853-39-4	Perfluorobenzophenone	362.1				x				**0.99**	**0.85**	**1.84**
176	86479-06-3	Hexaflumuron	461.1		x	x			x	x	**0.97**	**0.87**	**1.84**
177	3072-84-2	Tetrabromobiphenol A diglycidyl ether	656.0				x				**0.97**	**0.87**	**1.84**
178	68-36-0	Benzene, 1,4-bis(trichloromethyl)-	312.8				x				**0.94**	**0.90**	**1.84**
179	2274-74-0	Chlorfensulfide	352.1		x				x		**0.87**	**0.97**	**1.84**
180	335-65-9	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-Heptadecafluorooctane	420.1				x				**1.00**	**0.84**	**1.84**
181	133-14-2	Peroxide, bis(2,4-dichlorobenzoyl)	380.0				x				**0.88**	**0.96**	**1.84**
182	559-74-0	FRIEDELIN	426.7				x				**0.96**	**0.88**	**1.84**
183	93776-16-0	bis(2-hydroxyethyl)-methyl-(4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,15,15,15-pentacosafluoro-2-hydroxyp	796.3				x				**1.00**	**0.84**	**1.83**
184	3808-87-5	Bis(2,4,5-trichlorophenyl) disulfide	425.0				x				**0.96**	**0.88**	**1.83**
185	40088-47-9	Benzene, 1,1 -oxybis-, tetrabromo deriv.	485.8				x				**0.88**	**0.95**	**1.83**
186	84604-89-7	1,1'-Methylenebis(2,4-dichlorobenzene)	306.0				x				**0.85**	**0.98**	**1.83**
187	84604-90-0	1,1'-Methylenebis(2,6-dichlorobenzene)	306.0				x				**0.85**	**0.98**	**1.83**
188	2781-00-2	Peroxide, 1,4-phenylenebis(1-methylethylidene) bis (1,1-dimethylethyl)	338.5				x				**0.86**	**0.97**	**1.83**
189	25155-25-3	Peroxide, [1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[(1,1-dimethylethyl)	338.5				x				**0.86**	**0.97**	**1.83**
190	2212-81-9	1,3-bis(2-tert-butylperoxypropan-2-yl)benzene	338.5				x				**0.86**	**0.97**	**1.83**

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191	84297-66-5	Magnesium 1,2,3,4,5,6,7,8,13,13,14,14-dodecachloro-1,4,4a,4b,5,8,8a,12b-octahydro-11-sulphonato-1,4:5,8-dimethanotr	795.8				x				**1.00**	**0.83**	**1.83**
192	53097-59-9	2,3,4,5,6-Pentabromostyrene	498.6				x				**0.90**	**0.93**	**1.83**
193	94108-54-0	1-[4-(trifluoromethoxy)phenyl]sulfonyl-4-(trifluoromethyl)benzene	370.3				x				**0.92**	**0.91**	**1.83**
194	374-60-7	Perfluoro-n-butylcyclohexane	500.1				x				**1.00**	**0.83**	**1.83**
195	2227-13-6	Tetrasul (Animert)	324.1		x		x		x		**0.85**	**0.98**	**1.83**
196	26496-99-1	bis(2,4-dichlorophenyl) carbonate	352.0				x				**0.86**	**0.97**	**1.83**
197	68239-72-5	1-Pentanesulfonamide, 1,1,2,2,3,3,4,4,5,5,5-undecafluoro-N-(4-hydroxybutyl)-N-methyl-	435.3				x				**0.95**	**0.88**	**1.83**
198	67584-58-1	1-Propanaminium, N,N,N-trimethyl-3-[[(pentadecafluoroheptyl)sulfonyl]amino]-, iodide	549.3				x				**0.99**	**0.83**	**1.83**
199	1869-77-8	Glycine, N-ethyl-N- (heptadecafluorooctyl)sulfonyl -, ethyl ester	613.3				x				**0.97**	**0.86**	**1.82**
200	338-83-0	**Perfluamine**	521.1				x	x			**1.00**	**0.82**	**1.82**
201	85721-08-0	[2-chloro-5-(trifluoromethyl)phenyl]-(4-fluorophenyl)methanone	302.7				x				**0.90**	**0.93**	**1.82**
202	28655-71-2	**HEPTACHLOROBIPHENYL**	395.3				x				**0.97**	**0.86**	**1.82**
203	335-76-2	Decanoic acid, nonadecafluoro-	513.1				x				**0.89**	**0.93**	**1.82**
204	77549-03-2	6-Chloro-3-(4-chlorophenyl)-2,4-bis(2-fluorophenyl)-3,4-dihydroquinazolin-4-ol	481.3				x				**0.98**	**0.85**	**1.82**
205	27607-36-9	2-[3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl(2-hydroxyethyl)amino]ethanol	551.2				x				**0.99**	**0.83**	**1.82**
206	72-54-8	p,p'-DDD	320.0		x		x				**0.85**	**0.97**	**1.82**
207	1735-37-1	Bis(4-(trifluoromethoxy)phenyl) sulphone	386.3				x				**0.93**	**0.89**	**1.82**
208	67939-88-2	1-Octanesulfonamide, N-[3-(dimethylamino)propyl]-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-, monohydrochlorid	620.8				x				**1.00**	**0.83**	**1.82**
209	335-66-0	Octanoyl fluoride, pentadecafluoro-	402.1				x				**0.99**	**0.83**	**1.82**
210	53-19-0	Mitotane, o,p'-DDD	320.0				x	x			**0.85**	**0.97**	**1.82**
211	67923-41-5	3H-Pyrazol-3-one, 2-(4-chlorophenyl)-4- 4-chloro-2-(trifluoromethyl)phenyl azo -2,4-dihydro-5-methyl-	415.2				x				**0.95**	**0.87**	**1.82**
212	94133-66-1	1,3-Dichloro-9-methyl-6-(trifluoromethyl)phenanthrene	329.1				x				**0.89**	**0.93**	**1.82**
213	4162-45-2	Ethanol, 2,2 -[(1-methylethylidene)bis[(2,6-dibromo-4,1-phenylene)oxy]]bis-	632.0				x				**0.93**	**0.89**	**1.82**
214	16834-13-2	21H,23H-Porphine, 5,10,15,20-tetra-4-pyridinyl-	618.7				x				**0.96**	**0.86**	**1.82**
215	68901-25-7	1-Naphthalenesulfonic acid, 6-diazo-5,6-dihydro-5-oxo-, 1,1'-(thiodi-1,2-naphthalenediyl) ester	1279.2				x				**0.99**	**0.82**	**1.81**
216	85720-79-2	2,3-dichloro-1,1,1,2,3,4,5,5,5-nonafluoro-4-(trifluoromethyl)pentane	371.0				x				**1.00**	**0.81**	**1.81**
217	375-88-2	Heptane, 1-bromo-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-	449.0				x				**1.00**	**0.81**	**1.81**
218	72-55-9	**p,p'-DDE**	318.0				x				**0.82**	**0.99**	**1.81**
219	68679-99-2	**p,p'-DDE**	318.0				x				**0.82**	**0.99**	**1.81**
220	3311-94-2	1,1'-(4-Chloro-1-butenylidene)bis(4-fluorobenzene)	278.7				x				**0.85**	**0.97**	**1.81**
221	68227-99-6	4-(Methyl((undecafluoropentyl)sulphonyl)amino)butyl acrylate	489.3				x				**0.96**	**0.85**	**1.81**
222	67906-41-6	1-Heptanesulfonamide, N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-N-2-propenyl-	517.3				x				**0.93**	**0.88**	**1.81**
223	335-71-7	1-Heptanesulfonyl fluoride, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-	452.1				x				**1.00**	**0.81**	**1.81**
224	74592-66-8	3,5,5-Trimethylhexyl 2,4,5-trichlorophenoxyacetate	381.7				x				**0.86**	**0.95**	**1.81**
225	39569-21-6	TETRABROMO-2-CHLOROTOLUENE	442.2				x				**0.91**	**0.90**	**1.81**
226	1825-19-0	**PENTACHLORO(METHYLTHIO)BENZENE**	296.4				x				**0.88**	**0.93**	**1.81**
227	3424-82-6	1-(2-Chlorophenyl)-1-(4-chlorophenyl)- 2,2-dichloroethylene	318.0				x				**0.82**	**0.99**	**1.81**
228	2592-62-3	Bayer 38920; 6,7,8,9,10,10-Hexachloro-1,5,5a,6,9,9a-hexahydro-3-methyl-6,9-methano-2,4-benzdioxepin	386.9						x		**0.97**	**0.84**	**1.81**
229	375-95-1	Nonanoic acid, heptadecafluoro-	463.1				x				**0.84**	**0.97**	**1.81**

Rank	CAS RN	Name	MW	Ctgb	Alanwood	Biocide	EINECS	INN	PAN	EPA	P-score	B-score	PB-score
230	1336-36-3	**1,1'-Biphenyl, chloro derivs.**	292.0				x				**0.82**	**0.99**	**1.81**
231	2437-79-8	**2,2',4,4'-PCB**	292.0				x				**0.82**	**0.99**	**1.81**
232	73000-03-0	Pentafluorophenyl-tert-butylmethylsilyl chloride	302.7				x				**0.92**	**0.89**	**1.81**
233	67584-60-5	2-Propenoic acid, 2-methyl-, 2- methyl (undecafluoropentyl)sulfonyl amino ethyl ester	475.3				x				**0.95**	**0.85**	**1.81**
234	87-83-2	Benzene, pentabromomethyl-	486.6				x				**0.91**	**0.89**	**1.81**
235	87-82-1	Benzene, hexabromo-	551.5				x				**0.94**	**0.87**	**1.81**
236	15742-62-8	Octanoyl fluoride, tetradecafluoro-7-(trifluoromethyl)-	452.1				x				**0.99**	**0.81**	**1.81**
237	4151-50-2	1-Octanesulfonamide, N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-	527.2		x	x	x		x	x	**0.93**	**0.87**	**1.81**
238	85118-26-9	3-Chloro-1-(4-fluorophenyl)-5-(trifluoromethyl)indan	314.7				x				**0.89**	**0.91**	**1.80**
239	10541-71-6	1,4-Dichloro-2-(trichloromethyl)benzene	264.4				x				**0.88**	**0.92**	**1.80**
240	13014-24-9	Benzene, 1,2-dichloro-4-(trichloromethyl)-	264.4				x				**0.88**	**0.92**	**1.80**
241	31904-18-4	1,2-Dichloro-3-(trichloromethyl)benzene	264.4				x				**0.88**	**0.92**	**1.80**
242	84613-97-8	1,2-Dichloro-3-(trichloromethyl)benzene	264.4				x				**0.88**	**0.92**	**1.80**
243	93776-14-8	(2-Carboxyethyl)-3-((4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-heptadecafluoro-2-hydroxyundecyl)amino)propyldimethylam	651.4				x				**0.99**	**0.81**	**1.80**
244	58138-08-2	Oxirane, 2-(3,5-dichlorophenyl)-2-(2,2,2-trichloroethyl)-	320.4		x				x		**0.94**	**0.86**	**1.80**
245	13014-18-1	Benzene, 2,4-dichloro-1-(trichloromethyl)-	264.4				x				**0.88**	**0.92**	**1.80**
246	545-48-2	**Erythrodiol**	442.7				x				**0.93**	**0.87**	**1.80**
247	55684-94-1	**HEXACHLORODIBENZOFURAN**	374.9						x		**0.94**	**0.85**	**1.80**
248	51787-79-2	1,1'-(4-Iodobutylidene)bis(4-fluorobenzene)	372.2				x				**0.88**	**0.91**	**1.79**
249	67584-48-9	1-Hexanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-N-2-propenyl-	439.2				x				**0.85**	**0.95**	**1.79**
250	72-43-5	**Methoxychlor**	345.6		x	x	x				**0.88**	**0.91**	**1.79**

Substances which are discussed in the Results section have their names indicated in **boldface.**

Appendix 4 continued.

Properties and half-lives derived from QSAR calculations used to derive the PB-score, for the 250 highest scoring substances.

Rank	CAS RN	k OH (AOPv1.92)	t1/2(OH) hours	BIOWIN3	t1/2(water) hours	t1/2(soil) hours	log Kow (KowWin v1.67)	log Koa	log Kaw (HenryWin v.3.20)	BCFmax	t1/2 met. (BCFBAF v.3.00) days	BCF (met.)	TMF	BAF	LRTP-Pov (days)
1	93819-97-7	9.78E-11	3.94E+00	-1.3785	2759841	5519681	6.82	10.06	-3.24	4.55E+04	404.0	3.47E+04	8.4	2.91E+05	9.31E+04
2	2385-85-5	0.00E+00	3.85E+12	-2.2058	14436690	28873380	6.89	8.37	-1.48	4.42E+04	109.0	2.08E+04	9.9	2.05E+05	1.86E+06
3	39765-80-5	4.87E-12	7.91E+01	0.0225	167491	334982	6.35	9.34	-2.99	4.74E+04	218.0	2.95E+04	9.5	2.81E+05	1.44E+04
4	10386-84-2	6.89E-14	5.59E+03	-1.3359	2534440	5068881	7.14	9.17	-2.03	3.79E+04	90.4	1.75E+04	9.7	1.69E+05	9.34E+04
5	5566-34-7	6.46E-12	5.96E+01	0.0597	155482	310963	7.00	9.54	-2.54	4.17E+04	132.0	2.22E+04	9.3	2.06E+05	1.50E+04
6	18291-67-3	3.92E-12	9.83E+01	0.0507	158306	316611	7.13	9.50	-2.37	3.82E+04	110.0	1.94E+04	9.3	1.81E+05	1.52E+04
7	2550-75-6	4.77E-12	8.07E+01	0.2983	96479	192959	6.71	9.02	-2.31	4.71E+04	165.0	2.62E+04	9.8	2.57E+05	8.50E+03
8	57-74-9	5.92E-12	6.50E+01	0.2718	101731	203461	6.22	8.92	-2.70	4.56E+04	129.0	2.30E+04	9.8	2.26E+05	8.31E+03
9	5103-71-9	5.92E-12	6.50E+01	0.2718	101731	203461	6.22	8.92	-2.70	4.56E+04	129.0	2.30E+04	9.8	2.26E+05	8.31E+03
10	5103-74-2	5.92E-12	6.50E+01	0.2718	101731	203461	6.22	8.92	-2.70	4.56E+04	129.0	2.30E+04	9.8	2.26E+05	8.31E+03
11	93894-52-1	0.00E+00	3.85E+12	-0.9877	1263105	2526210	8.05	8.05	0.00	1.22E+04	291.0	1.09E+04	9.7	1.05E+05	1.90E+05
12	70281-93-5	8.30E-12	4.64E+01	0.3037	95443	190886	7.52	8.79	-1.27	2.62E+04	234.0	2.00E+04	9.9	1.97E+05	7.76E+03
13	97298-47-0	8.30E-12	4.64E+01	0.3037	95443	190886	7.52	8.79	-1.27	2.62E+04	234.0	2.00E+04	9.9	1.97E+05	7.76E+03
14	24448-09-7	1.61E-11	2.39E+01	0.1299	135115	270231	7.29	9.04	-1.75	3.34E+04	82.8	1.57E+04	9.8	1.54E+05	1.12E+04
15	1691-99-2	2.37E-11	1.62E+01	0.0990	143729	287458	7.78	9.41	-1.63	1.86E+04	114.0	1.28E+04	9.5	1.21E+05	1.42E+04
16	68239-75-8	2.47E-11	1.56E+01	0.0004	175060	350120	7.26	7.98	-0.72	3.43E+04	196.0	2.31E+04	9.6	2.21E+05	5.49E+03
17	8001-35-2	2.25E-12	1.71E+02	0.2629	103558	207115	5.78	9.39	-3.61	3.45E+04	64.3	1.38E+04	9.5	1.31E+05	1.02E+04
18	78974-42-2	2.39E-11	1.61E+01	-0.6245	610897	1221794	7.71	10.81	-3.10	2.05E+04	136.0	1.44E+04	6.4	9.17E+04	6.54E+04
19	18106-12-2	1.86E-11	2.07E+01	0.5667	56403	112807	6.03	9.23	-3.20	4.16E+04	104.0	1.97E+04	9.6	1.90E+05	5.79E+03
20	67584-62-7	1.59E-11	2.42E+01	0.5953	53268	106535	7.04	8.91	-1.87	4.07E+04	122.0	2.11E+04	9.9	2.08E+05	5.19E+03
21	68957-63-1	1.59E-11	2.42E+01	0.5953	53268	106535	7.04	8.91	-1.87	4.07E+04	122.0	2.11E+04	9.9	2.08E+05	5.19E+03
22	25935-14-2	1.15E-11	3.34E+01	0.0363	162931	325862	5.74	7.77	-2.03	3.32E+04	467.0	2.77E+04	9.3	2.59E+05	4.48E+03
23	2991-50-6	1.59E-11	2.42E+01	0.2727	101548	203095	8.01	9.16	-1.15	1.30E+04	323.0	1.17E+04	9.7	1.14E+05	9.83E+03
24	68298-89-5	1.89E-11	2.03E+01	0.3906	80216	160433	7.30	9.53	-2.23	3.31E+04	59.5	1.30E+04	9.3	1.21E+05	8.60E+03
25	18300-04-4	6.07E-12	6.34E+01	0.4796	67137	134273	6.44	9.95	-3.51	4.80E+04	59.4	1.48E+04	8.6	1.27E+05	7.55E+03
26	68412-68-0	2.80E-13	1.38E+03	0.0963	144507	289014	6.48	9.84	-3.36	4.82E+04	38.5	1.07E+04	8.8	9.46E+04	1.64E+04
27	13252-14-7	5.20E-13	7.41E+02	-0.1493	236164	472329	5.85	7.82	-1.97	3.66E+04	90.4	1.72E+04	9.4	1.62E+05	5.28E+03
28	309-00-2	6.46E-11	5.96E+00	0.7173	41735	83469	6.50	9.25	-2.75	4.82E+04	100.0	2.06E+04	9.6	1.98E+05	4.49E+03
29	465-73-6	6.55E-11	5.88E+00	0.7173	41735	83469	6.50	9.25	-2.75	4.82E+04	100.0	2.06E+04	9.6	1.98E+05	4.49E+03
30	68555-67-9	1.40E-13	2.75E+03	0.1315	134684	269367	6.27	8.72	-2.45	4.64E+04	36.5	1.02E+04	9.9	1.01E+05	1.07E+04
31	68631-02-7	6.04E-12	6.37E+01	0.8095	34707	69413	7.01	10.67	-3.66	4.15E+04	315.0	3.03E+04	6.8	2.06E+05	4.13E+03
32	68555-73-7	2.37E-11	1.62E+01	0.4216	75394	150788	6.81	9.16	-2.35	4.57E+04	43.2	1.16E+04	9.7	1.12E+05	7.37E+03
33	29082-74-4	1.07E-12	3.59E+02	0.8075	34846	69691	7.46	9.49	-2.03	2.80E+04	212.0	2.05E+04	9.4	1.92E+05	4.01E+03
34	2051-24-3	1.82E-14	2.12E+04	0.0312	164602	329203	8.27	8.69	-0.42	8.28E+03	939.0	8.08E+03	9.9	8.01E+04	1.57E+04

Rank	CAS RN	k OH (AOPv1.92)	t1/2(OH) hours	BIOWIN3	t1/2(water) hours	t1/2(soil) hours	log Kow (KowWin v1.67)	log Koa	log Kaw (HenryWin v.3.20)	BCFmax	t1/2 met. (BCFBAF v.3.00) days	BCF (met.)	TMF	BAF	LRTP-Pov (days)
35	14168-01-5	8.50E-12	4.53E+01	0.5211	61789	123578	6.08	8.17	-2.09	4.28E+04	75.3	1.66E+04	9.7	1.61E+05	4.02E+03
36	76-44-8	4.85E-11	7.95E+00	0.5256	61236	122471	6.10	8.02	-1.92	4.32E+04	78.3	1.70E+04	9.6	1.64E+05	3.69E+03
37	61660-12-6	2.47E-11	1.56E+01	-0.3222	333729	667457	8.23	8.23	0.00	8.91E+03	518.0	8.50E+03	9.8	8.32E+04	8.19E+03
38	4089-58-1	0.00E+00	3.85E+12	-0.0364	188430	376861	5.68	8.19	-2.51	3.13E+04	24.8	6.93E+03	9.8	6.77E+04	2.03E+04
39	68310-02-1	2.83E-11	1.36E+01	0.6579	46999	93998	7.79	9.90	-2.11	1.83E+04	88.7	1.16E+04	8.7	1.01E+05	5.47E+03
40	18052-83-0	2.37E-11	1.62E+01	0.5004	64401	128802	5.26	9.47	-4.21	1.87E+04	53.4	9.46E+03	9.4	8.88E+04	6.69E+03
41	1043-50-1	1.52E-12	2.54E+02	-1.6794	5037817	10075634	6.29	8.51	-2.22	4.67E+04	23.0	7.02E+03	9.9	6.95E+04	1.40E+04
42	68555-76-0	1.61E-11	2.39E+01	0.4526	70862	141723	6.32	8.80	-2.48	4.70E+04	31.3	9.07E+03	9.9	8.97E+04	6.08E+03
43	85284-15-7	1.49E-11	2.59E+01	-0.7402	769952	1539904	5.24	7.39	-2.15	1.82E+04	144.0	1.34E+04	8.8	1.18E+05	4.12E+03
44	68239-73-6	1.89E-11	2.03E+01	0.0680	152922	305844	8.27	9.78	-1.51	8.28E+03	157.0	7.22E+03	8.9	6.44E+04	1.67E+04
45	51936-55-1	1.11E-11	3.48E+01	0.3866	80861	161721	7.91	11.05	-3.14	1.53E+04	255.0	1.31E+04	5.5	7.20E+04	9.63E+03
46	40630-61-3	2.97E-11	1.30E+01	0.2236	112026	224051	6.72	9.79	-3.07	4.70E+04	25.6	7.69E+03	8.9	6.85E+04	1.17E+04
47	72-20-8	9.20E-12	4.19E+01	0.6733	45574	91147	5.20	8.59	-3.39	1.71E+04	103.0	1.17E+04	9.9	1.16E+05	3.97E+03
48	60-57-1	1.01E-11	3.82E+01	0.6733	45574	91147	5.20	8.59	-3.39	1.71E+04	103.0	1.17E+04	9.9	1.16E+05	3.97E+03
49	85665-66-3	1.90E-11	2.02E+01	0.8869	29729	59458	6.57	9.03	-2.46	4.81E+04	63.7	1.55E+04	9.8	1.52E+05	3.21E+03
50	93857-44-4	2.39E-11	1.61E+01	-0.0010	175551	351102	7.45	11.27	-3.82	2.84E+04	65.7	1.29E+04	4.7	6.03E+04	2.07E+04
51	475-26-3	6.01E-12	6.41E+01	0.8681	30868	61737	5.91	8.72	-2.81	3.83E+04	60.2	1.38E+04	9.9	1.37E+05	3.10E+03
52	13417-01-1	2.53E-11	1.52E+01	-0.3446	349020	698039	8.24	9.08	-0.84	8.75E+03	48.9	5.84E+03	9.8	5.70E+04	2.17E+04
53	1715-40-8	5.45E-12	7.07E+01	0.6825	44743	89485	5.90	8.36	-2.46	3.81E+04	38.9	1.02E+04	9.9	1.01E+05	3.63E+03
54	52584-45-9	6.83E-11	5.64E+00	-1.3637	2679346	5358693	6.15	6.67	-0.52	4.43E+04	472.0	3.51E+04	7.0	2.46E+05	2.25E+03
55	70729-63-4	6.83E-11	5.64E+00	-1.3637	2679346	5358693	6.15	6.67	-0.52	4.43E+04	472.0	3.51E+04	7.0	2.46E+05	2.25E+03
56	17202-41-4	1.40E-13	2.75E+03	-0.0339	187491	374981	7.24	6.87	0.37	3.49E+04	87.9	1.66E+04	7.6	1.25E+05	2.85E+03
57	18134-58-2	5.22E-12	7.38E+01	0.5641	56697	113395	6.47	9.26	-2.79	4.81E+04	23.1	7.08E+03	9.6	6.80E+04	5.92E+03
58	1506-15-6	1.41E-12	2.74E+02	1.0951	19604	39208	7.12	10.80	-3.68	3.85E+04	304.0	2.85E+04	6.4	1.82E+05	2.35E+03
59	94042-94-1	4.14E-11	9.29E+00	-0.4176	403884	807768	4.92	7.70	-2.78	1.09E+04	86.4	8.06E+03	9.3	7.47E+04	4.68E+03
60	67584-54-7	2.53E-11	1.52E+01	-0.0220	183081	366162	7.27	8.83	-1.56	3.40E+04	18.5	5.56E+03	9.9	5.49E+04	1.17E+04
61	754-91-6	0.00E+00	3.85E+12	0.0983	143930	287860	7.58	5.70	1.88	2.43E+04	84.4	1.35E+04	3.5	4.66E+04	8.69E+05
62	67584-53-6	1.59E-11	2.42E+01	0.9179	27942	55884	6.07	8.66	-2.59	4.25E+04	46.3	1.20E+04	9.9	1.18E+05	2.81E+03
63	68957-32-4	1.59E-11	2.42E+01	0.9179	27942	55884	6.07	8.66	-2.59	4.25E+04	46.3	1.20E+04	9.9	1.18E+05	2.81E+03
64	67939-96-2	3.19E-11	1.21E+01	0.2824	99597	199193	8.23	8.97	-0.74	8.91E+03	44.8	5.73E+03	9.8	5.63E+04	9.00E+03
65	68084-62-8	2.30E-11	1.67E+01	0.3134	93609	187218	7.68	8.62	-0.94	2.14E+04	23.6	6.07E+03	9.9	6.01E+04	6.94E+03
66	93894-55-4	6.20E-16	6.21E+05	0.7194	41560	83119	8.24	8.84	-0.60	8.75E+03	68.7	6.46E+03	9.9	6.38E+04	5.80E+03
67	55591-23-6	0.00E+00	3.85E+12	0.7007	43143	86287	8.00	6.25	1.75	1.32E+04	56.7	8.02E+03	5.6	4.52E+04	9.42E+04
68	66008-69-3	2.31E-11	1.67E+01	-0.0402	189868	379736	7.66	7.76	-0.10	2.19E+04	30.2	7.26E+03	9.3	6.77E+04	4.81E+03
69	94042-95-2	2.23E-11	1.73E+01	-2.0090	9739336	19478671	7.44	6.60	0.84	2.87E+04	2090.0	2.76E+04	6.8	1.88E+05	2.11E+03
70	94158-62-0	5.78E-11	6.66E+00	-0.4005	390305	780610	8.37	10.48	-2.11	6.87E+03	175.0	6.19E+03	7.3	4.55E+04	4.37E+04
71	423-50-7	0.00E+00	3.85E+12	0.7370	40122	80244	7.68	5.68	2.00	2.14E+04	94.5	1.31E+04	3.3	4.38E+04	2.72E+05
72	28680-45-7	4.19E-12	9.20E+01	0.6096	51766	103531	5.55	7.65	-2.10	2.72E+04	49.6	1.08E+04	9.2	9.89E+04	2.87E+03
73	59071-10-2	3.06E-11	1.26E+01	0.2824	99597	199193	8.17	8.99	-0.82	9.91E+03	32.5	5.36E+03	9.8	5.26E+04	9.04E+03

Rank	CAS RN	k OH (AOPv1.92)	t1/2(OH) hours	BIOWIN3	t1/2(water) hours	t1/2(soil) hours	log Kow (KowWin v1.67)	log Koa	log Kaw (HenryWin v.3.20)	BCFmax	t1/2 met. (BCFBAF v.3.00) days	BCF (met.)	TMF	BAF	LRTP-Pov (days)
74	68239-74-7	1.89E-11	2.03E+01	0.7132	42078	84156	6.34	9.29	-2.95	4.73E+04	22.5	6.90E+03	9.6	6.61E+04	4.55E+03
75	94158-61-9	5.78E-11	6.66E+00	0.2230	112160	224320	8.10	10.93	-2.83	1.12E+04	84.6	8.18E+03	5.9	4.86E+04	1.33E+04
76	881-99-2	6.55E-14	5.88E+03	1.0445	21692	43383	5.80	9.09	-3.29	3.51E+04	44.5	1.10E+04	9.7	1.07E+05	2.52E+03
77	67906-70-1	3.95E-11	9.75E+00	0.5740	55586	111172	7.75	9.09	-1.34	1.94E+04	23.4	5.86E+03	9.7	5.72E+04	5.78E+03
78	55910-10-6	1.90E-11	2.02E+01	0.2417	108043	216086	8.50	9.52	-1.02	5.34E+03	445.0	5.16E+03	9.3	4.81E+04	1.17E+04
79	24407-09-8	2.15E-11	1.79E+01	-0.3334	341289	682577	8.10	7.93	0.17	1.12E+04	33.6	5.81E+03	9.5	5.54E+04	6.16E+03
80	789-02-6	3.44E-12	1.12E+02	1.1961	16018	32036	6.79	10.31	-3.52	4.60E+04	149.0	2.47E+04	7.8	1.93E+05	1.91E+03
81	33979-03-2	3.95E-13	9.75E+02	1.1621	17145	34291	7.55	8.54	-0.99	2.52E+04	456.0	2.19E+04	9.9	2.17E+05	1.85E+03
82	50-29-3	3.44E-12	1.12E+02	1.1961	16018	32036	6.91	10.38	-3.47	4.38E+04	161.0	2.49E+04	7.6	1.90E+05	1.91E+03
83	335-77-3	1.40E-13	2.75E+03	-0.3565	357426	714852	8.21	7.12	1.09	9.23E+03	232.0	8.31E+03	8.2	6.80E+04	3.79E+03
84	434-90-2	1.37E-13	2.81E+03	-1.6086	4372666	8745332	5.76	6.86	-1.10	3.38E+04	40.1	1.01E+04	7.5	7.62E+04	3.18E+03
85	2888-15-5	1.62E-12	2.38E+02	1.0562	21190	42380	7.88	10.37	-2.49	1.60E+04	175.0	1.28E+04	7.6	9.75E+04	2.53E+03
86	16090-14-5	1.32E-12	2.91E+02	0.8345	33014	66028	6.24	7.58	-1.34	4.59E+04	46.8	1.23E+04	9.1	1.12E+05	2.25E+03
87	7421-93-4	3.37E-11	1.14E+01	0.2800	100076	200152	4.80	8.57	-3.77	8.81E+03	35.6	5.22E+03	9.9	5.17E+04	6.11E+03
88	81613-60-7	6.40E-11	6.02E+00	0.8414	32561	65123	7.08	9.49	-2.41	3.96E+04	23.0	6.83E+03	9.4	6.39E+04	3.70E+03
89	42115-16-2	3.88E-12	9.92E+01	1.1357	18075	36150	6.89	11.06	-4.17	4.42E+04	92.2	1.89E+04	5.5	1.04E+05	2.16E+03
90	1335-87-1	1.87E-13	2.06E+03	1.2196	15283	30566	7.04	9.49	-2.45	4.07E+04	69.6	1.55E+04	9.4	1.45E+05	1.82E+03
91	1024-57-3	6.06E-12	6.36E+01	0.4815	66882	133764	4.98	8.05	-3.07	1.21E+04	33.7	6.04E+03	9.7	5.83E+04	3.79E+03
92	67939-61-1	3.47E-11	1.11E+01	0.5430	59141	118282	8.24	9.46	-1.22	8.75E+03	32.2	4.98E+03	9.4	4.68E+04	6.61E+03
93	59493-82-2	8.28E-12	4.65E+01	0.9472	26352	52703	7.21	7.24	-0.03	3.59E+04	97.1	1.77E+04	8.5	1.50E+05	1.78E+03
94	67584-61-6	3.19E-11	1.21E+01	0.6050	52244	104488	7.26	8.72	-1.46	3.43E+04	17.0	5.18E+03	9.9	5.13E+04	4.82E+03
95	50285-18-2	0.00E+00	3.85E+12	-1.2927	2324658	4649316	6.80	-1.24	8.04	4.59E+04	484.0	3.63E+04	-63.4	3.63E+04	1.28E+11
96	4236-15-1	3.42E-11	1.13E+01	0.0680	152922	305844	8.48	10.21	-1.73	5.55E+03	111.0	4.87E+03	8.0	3.92E+04	1.76E+04
97	68227-98-5	2.58E-11	1.49E+01	0.5740	55586	111172	7.70	9.11	-1.41	2.08E+04	17.0	4.72E+03	9.7	4.59E+04	5.80E+03
98	67525-36-4	6.90E-12	5.58E+01	1.1768	16649	33297	8.03	10.13	-2.10	1.26E+04	919.0	1.21E+04	8.2	9.98E+04	1.99E+03
99	1107-00-2	3.30E-12	1.17E+02	0.9794	24708	49416	5.59	11.12	-5.53	2.85E+04	57.4	1.20E+04	5.3	6.29E+04	2.92E+03
100	65294-20-4	2.80E-11	1.37E+01	0.8654	31035	62071	7.62	7.12	0.50	2.31E+04	93.1	1.37E+04	8.2	1.12E+05	1.86E+03
101	1782-06-5	1.14E-11	3.37E+01	0.5847	54409	108818	5.39	10.70	-5.31	2.24E+04	25.4	6.48E+03	6.7	4.34E+04	6.29E+03
102	34455-03-3	2.37E-11	1.62E+01	0.7442	39549	79097	5.85	8.92	-3.07	3.66E+04	16.3	5.05E+03	9.8	4.97E+04	3.99E+03
103	85665-64-1	3.42E-11	1.13E+01	0.7132	42078	84156	6.54	9.71	-3.17	4.82E+04	15.9	5.10E+03	9.0	4.61E+04	4.76E+03
104	2227-17-0	7.86E-13	4.90E+02	-0.0058	177244	354488	8.39	11.04	-2.65	6.61E+03	685.0	6.44E+03	5.5	3.57E+04	2.12E+04
105	2234-13-1	3.84E-14	1.00E+04	0.6542	47348	94696	8.50	10.03	-1.53	5.34E+03	218.0	5.00E+03	8.4	4.22E+04	5.68E+03
106	28031-44-9	5.08E-11	7.59E+00	0.3229	91847	183695	6.99	21.50	-14.51	4.20E+04	823.0	3.68E+04	-114.9	3.68E+04	1.10E+04
107	32241-08-0	8.48E-14	4.54E+03	0.9369	26900	53800	8.20	10.78	-2.58	9.40E+03	167.0	8.13E+03	6.4	5.23E+04	3.23E+03
108	68555-66-8	1.40E-13	2.75E+03	0.4541	70649	141299	5.31	8.48	-3.17	2.01E+04	13.8	3.97E+03	9.9	3.93E+04	6.16E+03
109	115-32-2	3.43E-12	1.12E+02	1.0235	22622	45244	5.02	10.03	-5.01	1.29E+04	37.4	6.58E+03	8.4	5.56E+04	2.63E+03
110	1735-48-4	0.00E+00	3.85E+12	-0.6692	668027	1336053	6.54	-0.78	7.32	4.82E+04	234.0	3.06E+04	-56.8	3.06E+04	6.08E+10
111	16557-94-1	5.20E-13	7.41E+02	0.9543	25980	51960	6.61	6.79	-0.18	4.80E+04	80.4	1.80E+04	7.4	1.33E+05	1.47E+03
112	68318-36-5	3.36E-11	1.15E+01	0.1111	140292	280585	6.73	19.20	-12.47	4.69E+04	294.0	3.25E+04	-74.2	3.25E+04	1.68E+04

Rank	CAS RN	k OH (AOPv1.92)	t1/2(OH) hours	BIOWIN3	t1/2(water) hours	t1/2(soil) hours	log Kow (KowWin v1.67)	log Koa	log Kaw (HenryWin v.3.20)	BCFmax	t1/2 met. (BCFBAF v.3.00) days	BCF (met.)	TMF	BAF	LRTP-Pov (days)
113	25268-77-3	2.30E-11	1.67E+01	-0.0093	178489	356978	8.65	8.87	-0.22	3.94E+03	62.4	3.35E+03	9.9	3.31E+04	1.25E+04
114	69013-34-9	1.04E-10	3.71E+00	-1.8088	6525861	13051722	7.31	15.28	-7.97	3.28E+04	885.0	2.97E+04	-23.3	2.97E+04	7.83E+05
115	1893-52-3	3.06E-11	1.26E+01	0.6050	52244	104488	7.21	8.75	-1.54	3.59E+04	12.3	3.93E+03	9.9	3.89E+04	4.85E+03
116	1763-23-1	1.40E-13	2.75E+03	0.2887	98350	196699	6.28	6.63	-0.35	4.65E+04	33.2	9.49E+03	6.9	6.53E+04	2.05E+03
117	3734-48-3	6.30E-11	6.11E+00	0.7749	37193	74387	5.44	7.13	-1.69	2.38E+04	31.8	7.72E+03	8.2	6.34E+04	1.99E+03
118	25429-29-2	3.35E-13	1.15E+03	1.4448	9741	19482	6.98	9.40	-2.42	4.22E+04	288.0	3.00E+04	9.5	2.84E+05	1.16E+03
119	3658-57-9	5.20E-13	7.41E+02	0.3309	90390	180779	6.87	6.33	0.54	4.46E+04	166.0	2.55E+04	5.9	1.51E+05	1.29E+03
120	83721-47-5	3.49E-12	1.10E+02	0.8963	29175	58351	6.20	11.33	-5.13	4.53E+04	33.3	9.46E+03	4.4	4.18E+04	3.47E+03
121	94248-26-7	4.51E-12	8.54E+01	0.8963	29175	58351	6.20	11.33	-5.13	4.53E+04	33.3	9.46E+03	4.4	4.18E+04	3.47E+03
122	55485-74-0	1.84E-11	2.09E+01	0.5074	63506	127011	5.01	8.11	-3.10	1.27E+04	16.7	4.07E+03	9.7	3.95E+04	3.80E+03
123	68957-54-0	1.32E-11	2.92E+01	0.3089	94455	188911	7.82	7.06	0.76	1.75E+04	24.1	5.79E+03	8.0	4.66E+04	2.69E+03
124	3883-86-1	2.37E-13	1.63E+03	-0.7152	732401	1464802	5.36	6.60	-1.24	2.15E+04	35.8	8.04E+03	6.8	5.46E+04	2.18E+03
125	56860-12-9	8.49E-12	4.54E+01	1.1980	15957	31915	6.00	8.90	-2.90	4.08E+04	22.7	6.79E+03	9.9	6.70E+04	1.78E+03
126	53494-70-5	1.18E-11	3.27E+01	0.4474	71602	143205	4.99	11.07	-6.08	1.23E+04	31.0	5.84E+03	5.4	3.17E+04	8.04E+03
127	85118-22-5	2.44E-12	1.58E+02	1.1578	17293	34587	5.97	7.52	-1.55	4.00E+04	37.4	1.01E+04	9.0	9.03E+04	1.46E+03
128	68227-97-4	2.58E-11	1.49E+01	0.2514	105967	211934	8.66	9.35	-0.69	3.86E+03	44.8	3.12E+03	9.5	2.96E+04	1.10E+04
129	34598-33-9	1.40E-12	2.75E+02	0.4784	67298	134596	8.25	6.71	1.54	8.59E+03	378.0	8.08E+03	7.1	5.77E+04	1.91E+03
130	42115-15-1	3.23E-11	1.19E+01	1.4309	10015	20031	6.14	8.56	-2.42	4.41E+04	115.0	2.13E+04	9.9	2.11E+05	1.11E+03
131	67906-40-5	3.47E-11	1.11E+01	0.8656	31023	62046	7.28	9.22	-1.94	3.37E+04	12.2	3.88E+03	9.7	3.74E+04	3.46E+03
132	34482-99-0	6.67E-11	5.77E+00	1.0295	22352	44705	4.98	9.07	-4.09	1.21E+04	20.6	4.59E+03	9.8	4.48E+04	2.45E+03
133	69661-30-9	0.00E+00	3.85E+12	-1.5754	4091751	8183501	7.22	2.97	4.25	3.56E+04	264.0	2.59E+04	-14.2	2.59E+04	1.16E+10
134	67939-36-0	3.95E-11	9.75E+00	0.2514	105967	211934	8.72	9.34	-0.62	3.41E+03	61.8	2.96E+03	9.5	2.82E+04	1.10E+04
135	62601-17-6	2.92E-12	1.32E+02	1.2618	14046	28092	6.07	9.37	-3.30	4.25E+04	21.2	6.46E+03	9.5	6.14E+04	1.64E+03
136	297-78-9	5.55E-12	6.94E+01	0.2588	104410	208821	4.51	10.13	-5.62	5.07E+03	28.8	3.40E+03	8.2	2.80E+04	1.04E+04
137	73353-25-0	5.85E-11	6.58E+00	-0.3415	346862	693725	6.41	24.31	-17.90	4.79E+04	156.0	2.58E+04	-175.1	2.58E+04	4.13E+04
138	68555-75-9	1.61E-11	2.39E+01	0.7752	37171	74342	5.36	8.56	-3.20	2.15E+04	11.9	3.56E+03	9.9	3.53E+04	3.38E+03
139	1544-19-0	5.19E-11	7.42E+00	1.5000	8723	17445	7.41	8.69	-1.28	2.96E+04	158.0	1.95E+04	9.9	1.93E+05	9.96E+02
140	32534-81-9	5.50E-13	7.00E+02	1.2132	15480	30959	6.84	11.16	-4.32	4.52E+04	32.1	9.18E+03	5.1	4.69E+04	1.85E+03
141	76784-42-4	1.78E-11	2.17E+01	0.3757	82643	165286	5.00	10.17	-5.17	1.25E+04	12.3	3.26E+03	8.1	2.65E+04	8.97E+03
142	94159-85-0	2.15E-11	1.79E+01	-0.0408	190096	380192	7.04	8.35	-1.31	4.07E+04	8.2	2.74E+03	9.8	2.70E+04	7.61E+03
143	5736-49-2	1.11E-12	3.47E+02	-1.7850	6222507	12445014	6.01	7.99	-1.98	4.11E+04	8.5	2.83E+03	9.6	2.71E+04	7.29E+03
144	1652-63-7	2.66E-11	1.45E+01	-0.1253	225096	450193	7.27	16.25	-8.98	3.40E+04	239.0	2.44E+04	-33.8	2.44E+04	2.70E+04
145	53542-48-6	2.66E-11	1.45E+01	1.2339	14852	29704	7.08	9.44	-2.36	3.96E+04	16.6	5.18E+03	9.4	4.88E+04	1.74E+03
146	51800-99-8	9.78E-12	3.94E+01	1.0232	22636	45271	5.61	8.99	-3.38	2.91E+04	12.1	3.78E+03	9.8	3.71E+04	2.48E+03
147	94349-23-2	3.94E-11	9.77E+00	1.5008	8709	17417	6.24	8.83	-2.59	4.59E+04	70.9	1.64E+04	9.9	1.62E+05	1.00E+03
148	335-57-9	0.00E+00	3.85E+12	0.2551	105186	210372	6.99	0.39	6.60	4.20E+04	145.0	2.32E+04	-41.2	2.32E+04	1.12E+10
149	26604-52-4	2.60E-12	1.48E+02	0.6068	52056	104113	5.52	10.86	-5.34	2.63E+04	14.9	4.45E+03	6.2	2.75E+04	6.07E+03
150	2172-49-8	5.01E-12	7.68E+01	1.4299	10035	20071	6.45	11.56	-5.11	4.81E+04	135.0	2.41E+04	3.4	8.32E+04	1.20E+03
151	94159-86-1	5.16E-11	7.46E+00	0.2031	116714	233428	7.54	6.30	1.24	2.55E+04	84.4	1.39E+04	5.8	8.05E+04	1.21E+03

Rank	CAS RN	k OH (AOPv1.92)	t1/2(OH) hours	BIOWIN3	t1/2(water) hours	t1/2(soil) hours	log Kow (KowWin v1.67)	log Koa	log Kaw (HenryWin v.3.20)	BCFmax	t1/2 met. (BCFBAF v.3.00) days	BCF (met.)	TMF	BAF	LRTP-Pov (days)
152	67584-57-0	2.30E-11	1.67E+01	0.6360	49103	98207	6.72	8.38	-1.66	4.70E+04	8.9	3.00E+03	9.9	2.96E+04	3.92E+03
153	68298-10-2	1.35E-11	2.85E+01	0.2438	107590	215180	8.79	8.39	0.40	2.95E+03	80.5	2.67E+03	9.9	2.64E+04	6.48E+03
154	375-81-5	0.00E+00	3.85E+12	1.0596	21046	42093	6.72	5.44	1.28	4.70E+04	35.8	1.01E+04	2.2	2.25E+04	2.27E+05
155	34367-37-8	1.99E-11	1.94E+01	1.3541	11678	23357	5.16	8.65	-3.49	1.61E+04	31.3	6.62E+03	9.9	6.56E+04	1.29E+03
156	87996-57-4	1.99E-11	1.94E+01	1.3541	11678	23357	5.16	8.65	-3.49	1.61E+04	31.3	6.62E+03	9.9	6.56E+04	1.29E+03
157	83721-46-4	5.05E-12	7.62E+01	1.1790	16576	33151	5.56	10.56	-5.00	2.75E+04	20.0	5.70E+03	7.1	4.05E+04	1.97E+03
158	127-90-2	1.03E-12	3.74E+02	0.5461	58776	117551	5.10	9.69	-4.59	1.47E+04	9.9	2.86E+03	9.1	2.59E+04	6.52E+03
159	83929-68-4	3.30E-11	1.17E+01	1.4973	8770	17540	7.03	10.35	-3.32	4.10E+04	52.0	1.28E+04	7.7	9.85E+04	1.05E+03
160	1321-64-8	4.13E-13	9.32E+02	1.5023	8683	17365	6.39	8.71	-2.32	4.77E+04	41.8	1.14E+04	9.9	1.13E+05	1.00E+03
161	67584-49-0	3.50E-11	1.10E+01	0.3324	90119	180237	7.93	6.31	1.62	1.48E+04	134.0	1.13E+04	5.9	6.64E+04	1.21E+03
162	76253-60-6	5.52E-12	6.97E+01	1.4674	9310	18621	7.13	9.88	-2.75	3.82E+04	33.6	9.17E+03	8.7	8.01E+04	1.11E+03
163	143-50-0	0.00E+00	3.85E+12	-1.5484	3876656	7753312	5.41	11.07	-5.66	2.29E+04	13.2	3.93E+03	5.4	2.14E+04	4.25E+05
164	36065-30-2	6.52E-12	5.91E+01	1.3751	11198	22396	6.79	11.38	-4.59	4.60E+04	50.5	1.30E+04	4.2	5.48E+04	1.34E+03
165	67906-73-4	3.95E-11	9.75E+00	0.8966	29158	58316	6.79	8.85	-2.06	4.60E+04	8.9	2.97E+03	9.9	2.93E+04	3.06E+03
166	51032-47-4	9.86E-12	3.90E+01	-0.1355	229735	459471	6.60	11.81	-5.21	4.80E+04	32.6	9.41E+03	2.3	2.18E+04	2.73E+04
167	3389-71-7	4.66E-11	8.27E+00	0.8634	31160	62320	5.15	6.86	-1.71	1.59E+04	24.9	5.72E+03	7.5	4.31E+04	1.59E+03
168	67584-52-5	1.59E-11	2.42E+01	1.2406	14654	29308	5.11	8.42	-3.31	1.49E+04	17.5	4.42E+03	9.9	4.37E+04	1.53E+03
169	68957-31-3	1.59E-11	2.42E+01	1.2406	14654	29308	5.11	8.42	-3.31	1.49E+04	17.5	4.42E+03	9.9	4.37E+04	1.53E+03
170	118-74-1	1.69E-14	2.28E+04	1.3302	12250	24500	5.73	6.89	-1.16	3.29E+04	21.5	6.25E+03	7.6	4.76E+04	1.41E+03
171	50598-28-2	2.53E-11	1.52E+01	0.3006	96036	192073	6.31	8.59	-2.28	4.69E+04	7.0	2.39E+03	9.9	2.36E+04	6.61E+03
172	85721-09-1	2.40E-12	1.61E+02	1.3537	11688	23375	5.20	8.69	-3.49	1.71E+04	20.5	5.15E+03	9.9	5.10E+04	1.31E+03
173	94159-76-9	5.21E-11	7.40E+00	-1.5527	3910139	7820278	7.52	15.64	-8.12	2.62E+04	253.0	2.03E+04	-27.1	2.03E+04	4.69E+05
174	15720-98-6	0.00E+00	3.85E+12	-0.7747	824954	1649909	7.62	1.44	6.18	2.31E+04	456.0	2.03E+04	-29.1	2.03E+04	3.93E+10
175	853-39-4	7.96E-13	4.84E+02	-1.6930	5176726	10353453	5.15	8.58	-3.43	1.59E+04	6.9	2.15E+03	9.9	2.13E+04	1.58E+04
176	86479-06-3	2.10E-11	1.83E+01	0.6828	44716	89432	5.68	9.07	-3.39	3.13E+04	7.6	2.52E+03	9.8	2.46E+04	4.58E+03
177	3072-84-2	1.83E-11	2.11E+01	0.8598	31385	62770	7.40	17.74	-10.34	2.99E+04	490.0	2.56E+04	-52.6	2.56E+04	3.77E+03
178	68-36-0	4.81E-14	8.01E+03	1.0445	21692	43383	4.62	7.91	-3.29	6.29E+03	19.3	3.30E+03	9.5	3.14E+04	2.19E+03
179	2274-74-0	3.78E-12	1.02E+02	1.5947	7218	14435	6.67	10.32	-3.65	4.75E+04	73.1	1.69E+04	7.8	1.31E+05	8.64E+02
180	335-65-9	3.10E-16	1.24E+06	0.4852	66389	132778	7.34	0.92	6.42	3.18E+04	145.0	1.98E+04	-34.9	1.98E+04	7.47E+04
181	133-14-2	1.76E-12	2.19E+02	1.5330	8166	16331	6.01	10.37	-4.36	4.11E+04	38.9	1.04E+04	7.6	7.96E+04	9.76E+02
182	559-74-0	3.24E-11	1.19E+01	0.9609	25639	51279	8.77	9.92	-1.15	3.07E+03	470.0	3.02E+03	8.7	2.61E+04	3.05E+03
183	93776-16-0	5.21E-11	7.40E+00	-0.9292	1123639	2247279	7.26	16.10	-8.84	3.43E+04	122.0	1.92E+04	-32.1	1.92E+04	1.35E+05
184	3808-87-5	2.27E-10	1.70E+00	1.0204	22763	45526	8.17	11.65	-3.48	9.91E+03	230.0	8.85E+03	3.0	2.68E+04	2.73E+03
185	40088-47-9	1.50E-12	2.57E+02	1.5235	8322	16644	6.77	10.69	-3.92	4.63E+04	36.0	1.01E+04	6.7	6.80E+04	9.97E+02
186	84604-89-7	3.29E-12	1.17E+02	1.6217	6838	13676	6.59	8.82	-2.23	4.81E+04	63.2	1.54E+04	9.9	1.52E+05	7.94E+02
187	84604-90-0	3.29E-12	1.17E+02	1.6217	6838	13676	6.59	8.82	-2.23	4.81E+04	63.2	1.54E+04	9.9	1.52E+05	7.94E+02
188	2781-00-2	6.83E-12	5.64E+01	1.6027	7103	14206	7.34	9.74	-2.40	3.18E+04	55.6	1.23E+04	9.0	1.10E+05	8.47E+02
189	25155-25-3	6.83E-12	5.64E+01	1.6027	7103	14206	7.34	9.74	-2.40	3.18E+04	55.6	1.23E+04	9.0	1.10E+05	8.47E+02
190	2212-81-9	1.11E-11	3.46E+01	1.6027	7103	14206	7.34	9.74	-2.40	3.18E+04	55.6	1.23E+04	9.0	1.10E+05	8.47E+02

Rank	CAS RN	k OH (AOPv1.92)	t1/2(OH) hours	BIOWIN3	t1/2(water) hours	t1/2(soil) hours	log Kow (KowWin v1.67)	log Koa	log Kaw (HenryWin v.3.20)	BCFmax	t1/2 met. (BCFBAF v.3.00) days	BCF (met.)	TMF	BAF	LRTP-Pov (days)
191	84297-66-5	1.35E-11	2.85E+01	-1.8343	6867313	13734626	7.45	23.66	-16.21	2.84E+04	155.0	1.88E+04	-160.1	1.88E+04	8.24E+05
192	53097-59-9	2.63E-11	1.46E+01	1.4173	10292	20583	7.34	10.29	-2.95	3.18E+04	19.6	5.76E+03	7.8	4.52E+04	1.23E+03
193	94108-54-0	4.68E-12	8.23E+01	1.2969	13094	26187	4.62	9.00	-4.38	6.29E+03	26.1	3.76E+03	9.8	3.69E+04	1.48E+03
194	374-60-7	0.00E+00	3.85E+12	-0.3280	337622	675245	6.94	-0.87	7.81	4.31E+04	90.2	1.85E+04	-58.0	1.85E+04	3.54E+10
195	2227-13-6	4.42E-12	8.70E+01	1.6567	6376	12752	6.87	10.28	-3.41	4.46E+04	99.3	1.98E+04	7.9	1.56E+05	7.63E+02
196	26496-99-1	1.42E-12	2.72E+02	1.5949	7215	14430	5.78	8.76	-2.98	3.45E+04	39.1	9.98E+03	9.9	9.87E+04	8.36E+02
197	68239-72-5	1.89E-11	2.03E+01	1.0358	22072	44145	5.37	9.04	-3.67	2.18E+04	8.5	2.68E+03	9.8	2.62E+04	2.43E+03
198	67584-58-1	2.66E-11	1.45E+01	0.1973	118076	236152	6.30	16.00	-9.70	4.68E+04	90.3	1.92E+04	-31.0	1.92E+04	1.40E+04
199	1869-77-8	1.32E-11	2.92E+01	-0.0137	180067	360134	8.78	7.30	1.48	3.01E+03	63.8	2.66E+03	8.6	2.28E+04	3.61E+03
200	338-83-0	0.00E+00	3.85E+12	-1.0187	1343896	2687792	7.08	2.89	4.19	3.96E+04	90.9	1.79E+04	-14.9	1.79E+04	4.62E+09
201	85721-08-0	2.48E-12	1.55E+02	1.3814	11058	22115	4.95	8.17	-3.22	1.15E+04	21.5	4.61E+03	9.8	4.50E+04	1.16E+03
202	28655-71-2	1.05E-13	3.68E+03	0.8793	30184	60369	8.27	11.70	-3.43	8.28E+03	799.0	8.05E+03	2.8	2.26E+04	3.62E+03
203	335-76-2	5.20E-13	7.41E+02	0.2178	113333	226665	8.23	6.22	2.01	8.91E+03	526.0	8.50E+03	5.5	4.70E+04	1.12E+03
204	77549-03-2	5.21E-11	7.39E+00	0.6963	43525	87049	7.68	17.80	-10.12	2.14E+04	2400.0	2.08E+04	-53.4	2.08E+04	5.22E+03
205	27607-36-9	4.04E-11	9.53E+00	0.0483	159067	318135	6.66	8.93	-2.27	4.76E+04	5.6	1.93E+03	9.8	1.90E+04	1.11E+04
206	72-54-8	4.34E-12	8.86E+01	1.6575	6366	12731	6.02	9.59	-3.57	4.13E+04	58.8	1.40E+04	9.2	1.29E+05	7.58E+02
207	1735-37-1	9.19E-12	4.19E+01	1.2034	15786	31572	4.70	10.36	-5.66	7.32E+03	21.5	3.76E+03	7.7	2.88E+04	1.84E+03
208	67939-88-2	2.53E-11	1.52E+01	-0.1704	246344	492688	6.72	14.76	-8.04	4.70E+04	81.6	1.80E+04	-18.4	1.80E+04	2.94E+04
209	335-66-0	1.58E-15	2.44E+05	0.5249	61321	122643	7.48	1.36	6.12	2.74E+04	155.0	1.84E+04	-29.9	1.84E+04	1.47E+04
210	53-19-0	4.34E-12	8.86E+01	1.6575	6366	12731	5.87	9.35	-3.48	3.72E+04	53.0	1.26E+04	9.5	1.20E+05	7.55E+02
211	67923-41-5	5.02E-12	7.67E+01	1.0551	21237	42473	6.80	13.36	-6.56	4.59E+04	142.0	2.41E+04	-6.9	2.41E+04	2.54E+03
212	94133-66-1	9.69E-13	3.97E+02	1.4708	9247	18495	7.14	9.10	-1.96	3.79E+04	14.6	4.61E+03	9.7	4.49E+04	1.08E+03
213	4162-45-2	2.56E-11	1.50E+01	1.2501	14378	28757	6.78	17.92	-11.14	4.62E+04	207.0	2.85E+04	-55.1	2.85E+04	1.72E+03
214	16834-13-2	6.06E-10	6.35E-01	0.9997	23725	47450	6.71	33.18	-26.47	4.71E+04	122.0	2.27E+04	-444.0	2.27E+04	2.84E+03
215	68901-25-7	4.27E-10	9.02E-01	0.2823	99617	199233	7.58	38.93	-31.35	2.43E+04	188.0	1.79E+04	-681.4	1.79E+04	1.20E+04
216	85720-79-2	0.00E+00	3.85E+12	-0.1422	232835	465669	5.94	1.27	4.67	3.92E+04	81.3	1.67E+04	-30.9	1.67E+04	1.20E+10
217	375-88-2	0.00E+00	3.85E+12	0.4503	71188	142377	7.39	1.73	5.66	3.03E+04	104.0	1.67E+04	-26.0	1.67E+04	2.65E+09
218	72-55-9	7.43E-12	5.18E+01	1.7368	5432	10864	6.51	9.28	-2.77	4.82E+04	252.0	3.15E+04	9.6	3.02E+05	6.44E+02
219	68679-99-2	7.43E-12	5.18E+01	1.7368	5432	10864	6.51	9.28	-2.77	4.82E+04	252.0	3.15E+04	9.6	3.02E+05	6.44E+02
220	3311-94-2	9.23E-11	4.17E+00	1.5962	7196	14392	5.42	7.72	-2.30	2.32E+04	55.9	1.08E+04	9.3	1.00E+05	7.49E+02
221	68227-99-6	2.58E-11	1.49E+01	0.8966	29158	58316	6.73	8.86	-2.13	4.69E+04	6.4	2.20E+03	9.9	2.17E+04	3.07E+03
222	67906-41-6	4.38E-11	8.78E+00	0.2704	102016	204032	8.63	6.55	2.08	4.11E+03	346.0	3.98E+03	6.6	2.64E+04	1.84E+03
223	335-71-7	0.00E+00	3.85E+12	0.4144	76488	152975	8.65	5.93	2.72	3.94E+03	250.0	3.78E+03	4.4	1.66E+04	2.96E+05
224	74592-66-8	1.13E-11	3.40E+01	1.6058	7059	14118	7.29	10.35	-3.06	3.34E+04	31.9	8.53E+03	7.7	6.55E+04	8.45E+02
225	39569-21-6	1.91E-13	2.02E+03	1.3966	10727	21453	6.74	9.08	-2.34	4.68E+04	10.7	3.55E+03	9.8	3.46E+04	1.26E+03
226	1825-19-0	1.22E-12	3.17E+02	1.5111	8531	17062	5.82	8.66	-2.84	3.57E+04	15.7	4.87E+03	9.9	4.82E+04	9.75E+02
227	3424-82-6	7.43E-12	5.18E+01	1.7368	5432	10864	6.00	9.12	-3.12	4.08E+04	175.0	2.47E+04	9.7	2.41E+05	6.42E+02
228	2592-62-3	3.68E-11	1.05E+01	0.6514	47614	95228	4.31	9.23	-4.92	3.37E+03	13.8	2.01E+03	9.6	1.93E+04	4.56E+03
229	375-95-1	5.20E-13	7.41E+02	0.5404	59450	118899	7.27	5.98	1.29	3.40E+04	199.0	2.30E+04	4.6	1.06E+05	7.18E+02

Rank	CAS RN	k OH (AOPv1.92)	t1/2(OH) hours	BIOWIN3	t1/2(water) hours	t1/2(soil) hours	log Kow (KowWin v1.67)	log Koa	log Kaw (HenryWin v.3.20)	BCFmax	t1/2 met. (BCFBAF v.3.00) days	BCF (met.)	TMF	BAF	LRTP-Pov (days)
230	1336-36-3	8.13E-13	4.73E+02	1.7275	5534	11068	6.29	8.40	-2.11	4.67E+04	168.0	2.63E+04	9.9	2.60E+05	6.34E+02
231	2437-79-8	8.13E-13	4.73E+02	1.7275	5534	11068	6.29	8.40	-2.11	4.67E+04	168.0	2.63E+04	9.9	2.60E+05	6.34E+02
232	73000-03-0	1.94E-12	1.99E+02	0.1101	140573	281146	6.26	6.42	-0.16	4.63E+04	14.7	4.74E+03	6.2	2.95E+04	1.47E+03
233	67584-60-5	3.19E-11	1.21E+01	0.9276	27405	54810	6.30	8.48	-2.18	4.68E+04	6.4	2.20E+03	9.9	2.17E+04	2.64E+03
234	87-83-2	1.85E-13	2.08E+03	1.3690	11335	22671	6.99	9.60	-2.61	4.20E+04	10.2	3.37E+03	9.2	3.10E+04	1.35E+03
235	87-82-1	1.15E-14	3.36E+04	1.1644	17067	34133	6.07	9.13	-3.06	4.25E+04	7.3	2.48E+03	9.7	2.41E+04	2.02E+03
236	15742-62-8	1.58E-15	2.44E+05	-0.0985	213349	426698	7.74	0.90	6.84	1.97E+04	320.0	1.68E+04	-35.1	1.68E+04	1.47E+04
237	4151-50-2	8.85E-12	4.35E+01	0.0363	162931	325862	8.54	6.20	2.34	4.93E+03	262.0	4.68E+03	5.4	2.55E+04	1.77E+03
238	85118-26-9	5.91E-12	6.51E+01	1.3358	12114	24227	5.93	7.27	-1.34	3.89E+04	14.3	4.54E+03	8.5	3.86E+04	1.07E+03
239	10541-71-6	7.34E-14	5.25E+03	1.4701	9260	18520	5.18	7.41	-2.23	1.66E+04	19.5	4.93E+03	8.8	4.33E+04	9.85E+02
240	13014-24-9	7.34E-14	5.25E+03	1.4701	9260	18520	5.18	7.41	-2.23	1.66E+04	19.5	4.93E+03	8.8	4.33E+04	9.85E+02
241	31904-18-4	7.34E-14	5.25E+03	1.4701	9260	18520	5.18	7.41	-2.23	1.66E+04	19.5	4.93E+03	8.8	4.33E+04	9.85E+02
242	84613-97-8	7.34E-14	5.25E+03	1.4701	9260	18520	5.18	7.41	-2.23	1.66E+04	19.5	4.93E+03	8.8	4.33E+04	9.85E+02
243	93776-14-8	5.85E-11	6.58E+00	0.2820	99676	199353	6.15	24.77	-18.62	4.43E+04	75.4	1.68E+04	-186.1	1.68E+04	1.18E+04
244	58138-08-2	2.75E-12	1.40E+02	1.1254	18451	36902	5.18	9.96	-4.78	1.66E+04	8.8	2.64E+03	8.6	2.27E+04	2.17E+03
245	13014-18-1	1.77E-13	2.18E+03	1.4701	9260	18520	5.18	7.41	-2.23	1.66E+04	19.5	4.93E+03	8.8	4.33E+04	9.45E+02
246	545-48-2	1.27E-10	3.04E+00	1.2680	13873	27746	8.13	11.72	-3.59	1.06E+04	189.0	9.19E+03	2.7	2.52E+04	1.67E+03
247	55684-94-1	5.20E-14	7.41E+03	1.1312	18238	36477	7.58	11.04	-3.46	2.43E+04	13.1	3.94E+03	5.5	2.18E+04	2.19E+03
248	51787-79-2	1.08E-11	3.56E+01	1.4879	8936	17873	6.29	8.62	-2.33	4.67E+04	11.4	3.76E+03	9.9	3.73E+04	1.01E+03
249	67584-48-9	3.50E-11	1.10E+01	0.6551	47263	94526	6.96	6.07	0.90	4.27E+04	50.5	1.27E+04	4.9	6.30E+04	7.54E+02
250	72-43-5	5.35E-11	7.19E+00	1.5126	8506	17011	5.08	10.16	-5.08	1.42E+04	18.4	4.51E+03	8.1	3.68E+04	1.01E+03

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