Environment Agency

Evidence

Environmental prioritisation of low production volume substances under REACH: PBT screening

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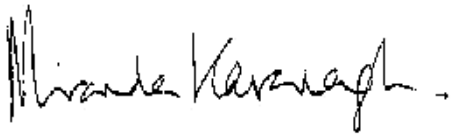

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Director of Evidence

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We thank the Health and Safety Executive (Douglas Gray) for providing a list of substances with appropriate health classifications.

Drafts of the report were presented to the Advisory Committee on Hazardous Substances for discussion at its meetings in June and December 2009. We thank them for their input.

Executive summary

The UK Chemicals Stakeholder Forum (UKCSF) developed prioritisation criteria for the nomination of substances to Annex XIV of the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) Regulation. In part, this report was commissioned to satisfy the request of the UKCSF to test these criteria against a list of substances, with a particular focus on chemicals that are potentially persistent, bioaccumulative and toxic (PBT) or 'very persistent and very bioaccumulative' (vPvB) according to the Annex XIII criteria of the REACH Regulation.

We began with a European list of almost 8000 substances supplied to the market by individual companies in the range 10 tonnes/year to 1000 tonnes/year ('low production volume' substances). An initial shortlist was compiled by screening the European list against existing databases on hazard classification, as well as against OSPAR and Canadian government sources. This shortlist was refined using quantitative structure–activity relationships to remove chemicals that did not appear to fit within the European Union PBT criteria. We then carried out a restricted search for additional measured property data, along with a search for readily available information on use pattern.

Thus, 184 substances were identified as candidates for further investigation. Of these, 103 are of high priority for further investigation (because they appear to meet the PBT and/or vPvB screening criteria and to have widespread dispersive exposures), and a further 66 are of medium priority and 15 of low priority (mainly because there appears to be no use). Of the high-priority group, 26 substances have structures or use patterns that suggest that they should be looked at first, although all substances will need to be examined further at some point to check that the assumptions we have made are appropriate.

We stress that none of the prioritised chemicals are confirmed PBT or vPvB substances at this stage. We did not scrutinise the raw data in any detail and, in particular, the suitability of the predictive techniques was not documented explicitly. Chemical companies may well have additional data in their possession that could lead to a change in the priority of any of these substances (whether through use pattern or properties), but no input was sought from them for this project. Since industry must compile and justify data sets under REACH, we recommend that this issue be revisited after the appropriate registration deadline has passed (the first of these is 1 December 2010).

Consequently, the output of this report is a working list, and it does not imply that an Annex XV dossier will be brought forward for any individual substance currently identified as of high or medium priority for further work. Rather, it is a contribution to further priority-setting activities by regulatory authorities in the UK and elsewhere in Europe, and for industry as they prepare for registration and test plan development under REACH.

At this stage, inorganic substances and complex substances for which no discrete structure can be identified were excluded. In addition, we did not consider other substances that may also be priorities in the future (for example, those that cause toxicity by interfering with endocrine systems).

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1 Introduction

The UK Chemicals Stakeholder Forum (UKCSF) agreed prioritisation criteria for substances for nomination to Annex XIV of the REACH Regulation[1] at its meetings in October 2008 and January 2009,[2] and these are provided in Appendix 1. This report was commissioned in part to satisfy the request of the UKCSF to test these criteria against a list of substances, with a particular focus on chemicals that are potentially persistent, bioaccumulative and toxic (PBT) or 'very persistent and very bioaccumulative' (vPvB) according to the Annex XIII criteria of the REACH Regulation (Table 1.1).

Table 1.1 PBT and vPvB criteria.

Property	PBT criteria	vPvB criteria
Persistence (P)	$T_{1/2}$ > 60 days in marine water, or $T_{1/2}$ > 40 days in fresh- or estuarine water, or $T_{1/2}$ > 180 days in marine sediment, or $T_{1/2}$ > 120 days in fresh- or estuarine sediment, or $T_{1/2}$ > 120 days in soil	$T_{1/2}$ > 60 days in marine, fresh- or estuarine water, or $T_{1/2}$ > 180 days in marine, fresh- or estuarine sediment, or $T_{1/2}$ > 180 days in soil
Bioaccumulation (B)	BCF > 2000 l/kg	BCF > 5000 l/kg
Toxicity (T)	NOEC < 0.01 mg/l for marine or freshwater organisms, or Substance is classified as carcinogenic (category 1 or 2), mutagenic (category 1 or 2) or toxic for reproduction (category 1, 2 or 3), or There is other evidence of chronic toxicity, as identified by the classifications: T, R48, or Xn, R48 according to Directive 67/548/EEC.	

BCF, bioconcentration factor; NOEC, no observed effect concentration; $T_{1/2}$, environmental half-life.

A European Commission PBT Working Group previously reviewed high production volume (HPV) substances [that is, those supplied in the European Union (EU) above 1000 tonnes/year] and notified new substances. In a separate initiative, a group of EU Member States has begun work to prioritise substances that are already classified as carcinogenic, mutagenic or reprotoxic (CMR). In this report we attempt to fill the gap left by these reviews, by screening so-called 'low' production volume (LPV) substances (produced or imported in Europe in quantities between 10 tonnes and 1000 tonnes/year during a three-year period in the early 1990s).

We searched existing sources of information on hazard classification and prioritisation of substances. These searches were used as the basis for identifying chemicals that are *possibly* PBT using the screening criteria of the REACH Technical Guidance

[1] Regulation (EC) No 1907/2206 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC.

[2] January 2009 minutes available at http://www.defra.gov.uk/environment/quality/chemicals/csf/090127/final-minutes-090127.pdf; October 2008 minutes available at http://webarchive.nationalarchives.gov.uk/20090306103114/http://www.defra.gov.uk/environment/chemicals/csf/081014/minutes-081014.pdf

Document (REACH TGD; ECHA, 2008; see Table 1.2). Substances already classified as CMR and/or with the risk phrase R48 (danger of serious damage to health by prolonged exposure) were also reviewed to see if the T criterion was met. We then carried out a search for further information to indicate the possible uses and commercial significance of the substances (with particular reference to the UK where possible) to identify those that would lead to widespread dispersive exposures.

Table 1.2 PBT screening criteria from REACH Technical Guidance.

Type of data	Criterion	Screening assignment
Persistence		
Ready biodegradability test	Readily biodegradable	Not P and not vP
Enhanced ready biodegradability test	Readily biodegradable	Not P and not vP
Specified tests on inherent biodegradability:		
Zahn-Wellens (OECD 302B)	≥70 % mineralisation (DOC removal) within seven days; log phase no longer than three days; removal before degradation occurs below 15%; no pre-adapted inoculum	Not P
MITI II test (OECD 302C)	≥70 % mineralisation (O_2 uptake) within 14 days; log phase no longer than three days; no pre-adapted inoculum	Not P
Biowin 2 (non-linear model prediction) and Biowin 3 (ultimate biodegradation time)	Does not biodegrade fast (probability < 0.5), and ultimate biodegradation timeframe prediction: ≥ months (value < 2.2)	P
Biowin 6 (MITI non-linear model prediction) and Biowin 3 (ultimate biodegradation time)	Does not biodegrade fast (probability < 0.5) and ultimate biodegradation timeframe prediction: ≥ months (value < 2.2)	P
Bioaccumulation		
Convincing evidence that a substance can biomagnify in the food chain (for example, field data)	For example, BMF > 1	B or vB, definitive assignment possible
Octanol–water partitioning coefficient (experimentally determined or estimated by QSAR)	Log K_{ow} ≥ 5	vB
	Log K_{ow} ≥ 4.5	B
Toxicity		
Short-term aquatic toxicity	EC_{50} or LC_{50} < 0.01 mg/l	T, criterion considered to be definitely fulfilled
	EC_{50} or LC_{50} < 0.1 mg/l	T
Avian toxicity (subchronic or chronic toxicity or toxic for reproduction)	NOEC < 30 mg/kg food	T

BMF, biomagnification factor; DOC, dissolved organic carbon; EC_{50}, concentration that causes a 50 per cent response; LC_{50}, concentration that causes 50 per cent lethality; OECD, Organisation for Economic Co-operation and Development; QSAR, quantitative structure–activity relationship.

The report does not consider inorganic substances and complex substances for which no discrete structure can be identified. Similarly degradation products that are not supplied as such are also excluded. Other substances (for example, those that cause toxicity by interfering with endocrine systems) may also be priorities in the future, but we did not consider such properties in this review.

The current Annex XIII criteria rely on measured environmental half-life and aquatic bioconcentration data. These are rarely available for LPV substances, so few, if any, substances identified in this review can be expected to be actual candidates for inclusion in Annex XIV at this time. Instead, the intention is to help companies prepare for registration, and to help the UK Government, including the UKCSF, to set priorities for future work.

2 Initial identification of candidate substances

2.1 Starting point

This project is based on the list of LPV substances in the European Chemical Substances Information System (ESIS)[3] database of the former European Chemicals Bureau (ECB). We obtained this by copying in sections from the ECB website to create a spreadsheet file. This file has details of 7829 substances, and consists of a list of Chemical Abstracts Service (CAS) and European Inventory of Existing Commercial Chemical Substances (EINECS) numbers and substance names. We recognise that this list may now be out of date. Nevertheless, it remains the most reliable list available for the purposes of this study.

2.2 Uses of existing classification or screening results

We decided to use the results of existing hazard classification and screening exercises to refine the initial list into a more manageable shortlist of possible candidate substances. To do this we compared the CAS numbers of the substances in the LPV list with the sources of information that are briefly summarised below.

- The Danish Environment Protection Agency (EPA) has produced a database for the self-classification of substances, using predicted properties (Danish EPA, 2001). The predictions were obtained using quantitative structure–activity relationship (QSAR) methods. These could be applied only to substances with unambiguous chemical structures (so-called 'discrete substances'). The methods were applied to 46,707 discrete substances included in EINECS (a list of all substances on the European market between 1971 and 1981). As far as possible, we excluded substances already classified by the EU. We also excluded inorganic substances. Substances were only included on the list if the predictive method gave a positive prediction of a property that met the classification criteria. We did not include substances for which the predictions were unreliable, nor those for which the predictions did not meet the classification criteria.

  The QSARs used in Danish EPA (2001) were a mixture of in-house and publicly available models. For aquatic toxicity, the multiple computer automated structure evaluation (M-CASE) system was used to develop a model for acute toxicity to fathead minnows. A number of models developed by the M-CASE system were used to predict mutagenicity; these were applied in a specific sequence, and an expert evaluation step was also included after application of the models. Biodegradation was predicted using the Syracuse BIOWIN program, based only on the linear equation for rapid or non-rapid biodegradation (Biowin 1). This was used to predict when a substance was not readily biodegradable. Finally, bioconcentration was predicted using the Syracuse BCFWIN program.

  We gave substances a suggested classification on the basis of the predicted values for aquatic toxicity, mutagenicity, persistence and accumulation. The criteria used

[3] http://ecb.jrc.ec.europa.eu/esis

for classification were those applied under the EU Dangerous Substances Directive[4] (for further information, see the Chemical Hazard, Information and Packaging for Supply Regulations[5]).

The database contains CAS and EINECS numbers, chemical names and the indicated classification for 20,624 substances. None of the predicted data values used as the basis for the classification are included. Hazard classification can be employed as a high-level screening tool because data on persistence, bioaccumulation and toxicity are used to define the environmental hazard. Substances classified as R50-53, or R53 with an appropriate health classification, may possibly be PBT. Substances with a classification of R53 alone could be vPvB, but the reason for applying the classification may relate to only one of these (persistence or accumulation), and not all of the source lists included this classification or equivalent. As a result, in this project we did not include substances with only an R53 classification.[6]

We compared the database to the LPV list, and 1850 matches were produced. This subset was screened for substances with the classification R50-53, to give 248 matches. We carried out a further screen for substances with the classification R51-53 plus any carcinogen or mutagen classifications (reproductive toxicity could not be considered, as this endpoint was not included in the Danish study). There are no predictions of carcinogenicity Category (Cat) 1 or 2 in the data set. The model used for mutagenicity could not distinguish between the different classes, and so all were reported as Cat 3 mutagens; 18 substances with R51-53 and Mut 3 were also in the LPV list. This gave a total of 266 substances.

- The N-Class database[7] contains the agreed EU classifications for substances and can be searched for particular classifications. It was searched for substances with the classification R50-53, which produced a list of 2463 substances. This includes a number of multiple entries. A comparison with the LPV list gave a total of 241 matches, which included 14 duplicates or triplicate entries (that is, the same substance with an older and newer classification, or a different name). At this stage, we removed inorganic substances from the list.

  A comparison of the two subsets of LPV substances with R50-53 showed only four substances common to both.

- A further list considered as an indicator of possible priority substances is the OSPAR list of substances of possible concern. We obtained this from the OSPAR website,[8] and compared it with the LPV list as above, which resulted in 83 hits. We compared these to the subsets obtained from the Danish and N-Class data sets, and found 49 of the OSPAR substances already listed in those subsets. These were left in the extracted lists, but are identified as OSPAR substances. For the substances from the OSPAR list not already included, we used an assessment of 'very toxic for ecotoxicity' from the OSPAR fact sheets to identify additional substances to include. Note that some of the substances are considered very toxic on the basis of predicted chronic toxicity, which is not necessarily comparable with the other lists.

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[4] Council Directive 67/548/EEC of 27 June 1967 on the approximation of laws, regulations and administrative provisions relating to the classification, packaging and labelling of dangerous substances.

[5] http://www.hse.gov.uk/chip/index.htm

[6] Substances classified as R52-53 could also have been considered, but the level of aquatic toxicity ($L(E)C_{50}$ > 10 mg/l) is unlikely to trigger the T criterion, and so to keep the list manageable these were ignored. This also applies to N-Class.

[7] http://apps.kemi.se/nclass/default.asp

[8] http://www.ospar.org/content/content.asp?menu=00120000000050_000000_000000

- The Canadian Government has carried out a categorisation of all of the substances on its Domestic Substance List[9] (DSL). This list contains approximately 22,400 substances in commercial use in Canada in 1984 to 1986. The methods used to carry out the categorisation are described by Environment Canada[10] and on the Health Canada website.[11] Although experimental data were used where available, the exercise made extensive use of QSAR models to predict persistence, bioaccumulation and toxicity. The substances from this categorisation of relevance to the current work are those identified as persistent, bioaccumulative and inherently toxic to non-human organisms (PBiT) and those persistent, bioaccumulative and inherently toxic to humans (PBiThuman). Note that the persistence and bioaccumulation criteria are not exactly the same as those used in REACH, but are similar.

  We screened the substances characterised as PBiT and PBiThuman against the LPV list, with 77 and 30 hits, respectively (with one common to both). When we compared these results with those from the screening of the Danish, N-Class and OSPAR lists above, we found 17 duplicates for the PBiT list and four for the PBiThuman list. We added the 85 unique results to the list of candidate substances.

- We also screened the LPV list against substances with health-based classifications relevant to the T criterion – CMR categories 1 and 2, Repro Cat. 3 and R48. The Health and Safety Executive (HSE) provided lists of substances with Repro Cat. 3 and R48 classifications. We also obtained a list of agreed CMR category 1 and 2 substances from the Europa website,[12] and screened these lists against the LPV list. We thus identified a further 58 substances, after removing those already included from the work described above.

With the above selection processes we identified a total of 666 substances for the initial shortlist.

2.3 'Persistent and bioaccumulative' screen

The criteria used for the various source lists (Danish EPA, N-Class, OSPAR, DSL and HSE) are not necessarily the same as those in the REACH TGD for PBT substances, either for actual data or for screening.[13] It was therefore necessary to perform a further assessment.

Firstly, we assumed that the presence of a substance on one of the source lists indicated that it was likely to meet the T criterion *at this stage of the process*. To assess the substances against the P and B criteria, we decided to calculate values using the EPI SUITE™ program and to assess these against the screening criteria in the REACH TGD. This is a screening-level tool developed by the US EPA, and consists of a variety of QSAR models.[14] While other models are available, it was not feasible to perform a comprehensive weight-of-evidence analysis for the purposes of this project. EPI SUITE™ is attractive because it is freely available and widely used, and so interested parties can easily check the calculations. In addition, it can be used in batch mode, and so it was cost-effective given the limited time available to screen each substance.

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9 http://www.ec.gc.ca/substances/ese/eng/dsl/dslprog.cfm

10 http://www.ec.gc.ca/substances/ese/eng/dsl/cat_criteria_process.cfm

11 http://www.hc-sc.gc.ca/ewh-semt/contaminants/existsub/index_e.html

12 http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2007:136:0003:0280:EN:PDF

13 For example, the OSPAR B criterion is log K_{ow} ≥ 4 or BCF ≥ 500. For the Canadian DSL, the persistence criteria include the air compartment (half-life ≥ 2 days); the numerical criteria for bioaccumulation are a bioaccumulation factor or BCF ≥ 5000 or log K_{ow} ≥ 5.

14 http://www.epa.gov/oppt/exposure/pubs/EPI SUITEdl.htm

We performed the calculations by entering the CAS number of the substance into the program (batch files were used). If there was no match to the CAS number database in the program, no automatic calculations were possible, and these substances were excluded. These were largely substances for which the name did not define the structure explicitly, but also included some metal salts of organic acids; they are listed in Appendix 4 and have not been reviewed further for this project. Note that CAS numbers were available for some metal salts of long-chain organic acids and these are included in the results.

We entered the following results from the EPI SUITE™ calculations into the spreadsheets for each of the subsets:

- three BIOWIN predictions (BIOWIN 2, 3 and 6);
- predicted log K_{ow};
- measured log K_{ow} if in the model database;
- predicted BCF;
- predicted solubility (from log K_{ow});
- measured solubility (if in the model database);
- ECOSAR™ class identified.

We used these values to screen the substances for persistence (P) and bioaccumulation (B). For biodegradation, the criteria in the REACH TGD for using the combination of the three BIOWIN predictions were used, as follows:

- If BIOWIN 3 is $\geq$ 2.2 and either BIOWIN 2 or BIOWIN 6 is $\geq$ 0.5, then the substance is not considered to be persistent.

The screening assessment of bioaccumulation uses the measured log K_{ow} value if available; otherwise the predicted value is used. The criteria values from the REACH TGD were used, as follows:

- log K_{ow} > 5, vB criterion met;
- log K_{ow} > 4.5, B criterion met.

We entered the predicted BCF values for possible future use, but they were not used in this exercise. These values are likely to differ from those that would be obtained using the BCF equations in the TGD, especially for higher log K_{ow} values. The solubility values were also not used; they may be of use in considering whether substances can demonstrate toxicity at concentrations below their solubility if the data are examined in more detail in the future.

Following the P and B screening, we extracted substances from the lists as:

- P + vB (PvB in the tables);
- P + B (PB in the tables).

A number of studies have previously been carried out by the Environment Agency on specific sectors of industry or on substances used for specific purposes. These cover flame retardants (Environment Agency, 2003), UV filters used in cosmetics (Environment Agency, 2008), fragrances (Environment Agency, in preparation) and alkylphenols (Environment Agency, 2005). These studies identified a number of priority

substances for further work in relation to their PBT properties. Those that are also LPVs were added to the list of candidate substances.[15]

The substances identified through the processes above are listed in Appendix 3. At this stage we allocated the substances a project code number, for example PvB1 for substances categorised as P and vB, and PB1 for substances categorised as P and B.

Note that the screen for persistence here is based only on the predicted biodegradability in aquatic ecosystems. Degradation by abiotic processes (for example, hydrolysis) or reaction may also be possible. This is indicated for a few substances in the fact sheets, but we did not undertake a systematic investigation of such possibilities for any substance.

Substances that have been the subject of a full assessment under programmes such as the EU Existing Substances Regulation (ESR) or the UK Co-ordinated Chemicals Risk Management Programme (CCRMP), or that have already been assessed by the EU PBT Working Group (EU PBT WG), were identified and removed from the main list. These substances are listed in Appendix 3, along with the reason for their removal. This first phase of the review gave a shortlist of 169 candidate PBT substances that have not already been assessed in detail by EU regulators.

[15] The criteria used in the individual reports do not necessarily match those in the REACH guidance. The reports were produced over the period of time when the criteria were being developed and methods to estimate the relevant properties were being agreed.

3 Further information and indications of commercial use

The second phase of the review was to seek readily available published property data and use pattern information (except for those substances identified from sector-specific studies, for which the equivalent information was gathered as part of the original study). Information collected through these steps was added to the screening results in fact sheets on each of the substances (which are provided as Appendix 2).

3.1 Property data

We conducted a brief search for experimental data on the substances identified in the first phase. This involved searching for the CAS numbers of the substances on the websites for the US HPV Challenge[16] (HPVIS) and the OECD HPV programmes,[17] the Japanese Chemical Risk Information Platform[18] and the Euras gold-standard bioconcentration (GSB) factor database.[19] Any information from these sites was used 'as found', and no attempt was made to check or validate it. Only experimental data were included; predicted values (even when different from those calculated for this study) were not. The data included in the fact sheets relate mainly to persistence and to accumulation, although some aquatic toxicity and physicochemical property data were also located. In a small number of cases the Environment Agency had additional information on properties, and these are mentioned in the fact sheets. However, this was not a systematic process.

3.1.1 Further consideration of effects data

The criteria used in the various source lists to identify substances as 'toxic' are not the same as those for classification as T for PBT under REACH.[20] For the substances identified in the first phase, we used the ECOSAR™ program to obtain predictions of toxicity to aquatic organisms. The calculations were based on the calculated log K_{ow} values from the KOWWIN program. The lowest chronic toxicity predictions were identified, and these are included in the fact sheets. The number and type of predicted values for each substance depends on the class of chemical to which the substance is assigned by the program. In selecting the lowest value, chronic values[21] (ChVs) for freshwater fish, invertebrates and algae were preferred. For the class of neutral organics, there is no chronic invertebrate prediction; instead, a 16-day EC_{50} value for *Daphnia* is predicted. For these substances, this value was considered along with the ChVs for fish and algae. For some classes there are either no chronic toxicity predictions or only chronic predictions for algae. In these cases we included the lowest

[16] http://www.epa.gov/chemrtk/hpvis/index.html
[17] http://cs3hq.oecd.org/scripts/hpv/
[18] http://www.safe.nite.go.jp/english/sougou/view/Disclaimer_en.faces
[19] http://ambit.sourceforge.net/euras/
[20] For example, the OSPAR T criterion is acute L(E)C_{50} ≤ 1 mg/l, long-term NOEC ≤ 0.1 mg/l or 'CMR or chronic toxicity'. The toxicity criteria for the Canadian DSL categorisation are broadly the same as those for OSPAR.
[21] The ChV is not the same as a NOEC value; it is equivalent to the geometric mean of the NOEC and LOEC. The predicted values from ECOSAR are in the form of ChV values, and were used as calculated to aid traceability.

acute toxicity prediction [L(E)C_{50}] in the tables (if relevant, that is when this is below the chronic algal value). Where only acute values were available and they were all above the T threshold, a result of *No prediction* is reported. The values included in the fact sheets were not used to change the identification of substances as 'T', but a note is included if the predicted chronic toxicity value is above the T threshold. The source of the identification as 'T' (the original classification and/or screening exercise) is indicated in the fact sheets in the ecotoxicity section.

3.2 Use pattern information

A number of different information sources were used to try to obtain information on the possible uses of the substances and whether they are in current use. We searched the confidential International Uniform Chemical Information Database (IUCLID 4) for each of the substances on the PvB and PB lists. The LPV list was derived from the IUCLID submissions and so all of the substances were found in the database. As the submissions for LPVs were completed by 1998, with limited updates up until 2000, this information does not necessarily reflect the current situation. Information on the use pattern and quantities produced or imported is considered confidential, and we have used it only to give an indication of where there is potential for exposure over a wide scale. The identities of companies that submitted IUCLID files is not confidential (they can be seen on the ESIS[22] database). However, the names and organisation of chemical companies have changed significantly over the ten years since the submissions and so it was not thought useful to include these as such; instead, a note is given in the fact sheets where a UK company was included.

We carried out a search of the web using Google®. The CAS number of each chemical was entered, with follow-ups using trade names if these were found in the initial screen of hits. In cases where the search returned a large number of hits, we appended 'use' or 'manufacturer' to the search term to find the required information. A few of the searches resulted in no matches, and some resulted in no English language matches, in which case no information was recorded. The information noted was the URL for companies that manufacture, supply, export or provide information on the corresponding chemicals. Only the results for UK-based companies are included in the fact sheets. No UK results were found for several of the chemicals for which the IUCLID search gave UK manufacturers. However, this does not necessarily mean that no UK companies currently manufacture the chemicals, and a note based on the IUCLID entry is included on the fact sheet. In general, there were very few results in the UK-only searches. We interpreted the results as showing that the substances could be in commerce if any sites that offered them for sale (or sites that linked to suppliers) were found anywhere in the world. A number of substances may only be available as laboratory-supply chemicals, but this could not be confirmed. Hence, in most cases no information from these searches is included on the fact sheets. The exception is where no suppliers were found at all; this is noted in the fact sheet under the potential for exposure.

A search for information in the *Kirk-Othmer Encyclopaedia of Chemical Technology* (Fourth Edition; various volumes and dates) was also carried out, and any appropriate use information included.

The information collected through the above searches is partly confidential, and so the full results of these searches are included in the confidential annex to this report.

[22] http://ecb.jrc.ec.europa.eu/esis/

4 Results

4.1 Overall results

The information from the sections above on each substance is summarised in a fact sheet on each, given in Appendix 2.

We gave the substances a basic rating of high, medium or low priority for further investigation, based on the data in the fact sheet. All substances have a high priority unless:

- No suppliers were located or the use is as an intermediate, in which case the substances are of medium priority. This is because there could be some dispersive uses, but they are likely to be minor. Further investigation may well indicate that these substances should have a lower priority.
- The substances do not meet the PBT or vPvB criteria on the basis of experimental data, in which case they are given a low priority.

A low-priority allocation should be considered as provisional pending checks on the original source of the experimental data.

Table 4.1, Table 4.2 and Table 4.3 list the substances assigned to each priority category.

As noted in the priority classification, in some cases the experimental data located through the processes described in Section 3 demonstrate that a substance does not match one or more of the criteria. The code numbers for substances not considered to be PBT or PvB on this basis are:

PvB: 2, 40, 63, 91, 108, 151, 152, 159

PB: 6, 20, 23, 35

Fact sheets for these substances are still included in Appendix 2, with an indication of the revised outcome.

There are also two instances in which the classification has changed as a result of experimental data; PvB21 becomes a PBT substance, and PB15 becomes a PvB substance. The fact sheets for these appear under their initial project code.

Table 4.1 High-priority substances.

Code no	CAS	Name
PvB1	10192-93-5	benzene, 1,1′-(1,2-diethyl-1,2-dimethyl-1,2-ethanediyl)bis-
PvB3	11028-42-5	cedrene
PvB11	139-60-6	1,4-benzenediamine, N,N′-bis(1-ethyl-3-methylpentyl)-
PvB12	1484-08-8	9H-carbazole, 9-butyl-
PvB13	15233-47-3	1,4-benzenediamine, N-(1-methylheptyl)-N′-phenyl-
PvB15	17540-75-9	phenol, 2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-
PvB17	1889-67-4	benzene, 1,1′-(1,1,2,2-tetramethyl-1,2-ethanediyl)bis-
PvB19	23593-75-1	1H-imidazole, 1-[(2-chlorophenyl)diphenylmethyl]-
PvB20	2422-91-5	benzene, 1,1′,1″-methylidynetris[4-isocyanato-
PvB21	25973-55-1	phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)-
PvB22	29312-59-2	benzenamine, 4-(2,6-diphenyl-4-pyridinyl)-N,N-dimethyl-
PvB23	29398-96-7	[1,1′-biphenyl]-4,4′-diamine, N,N′-bis(2,4-dinitrophenyl)-3,3′-dimethoxy-
PvB24	3081-01-4	1,4-benzenediamine, N-(1,4-dimethylpentyl)-N′-phenyl-
PvB25	3147-75-9	phenol, 2-(2H-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)-
PvB26	32388-55-9	ethanone, 1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)-, [3R-(3alpha,3abeta,7beta,8aalpha)]-
PvB27	3271-22-5	1,3,5-triazine, 2,4-dimethoxy-6-(1-pyrenyl)-
PvB28	3278-89-5	benzene, 1,3,5-tribromo-2-(2-propenyloxy)-
PvB29	335-57-9	heptane, hexadecafluoro-
PvB30	3407-42-9	cyclohexanol, 3-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)-
PvB31	355-42-0	hexane, tetradecafluoro-
PvB33	36437-37-3	phenol, 2-(2H-benzotriazol-2-yl)-4-(1,1-dimethylethyl)-6-(1-methylpropyl)-
PvB35	3846-71-7	phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)-
PvB37	3864-99-1	phenol, 2-(5-chloro-2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)-
PvB39	4130-42-1	phenol, 2,6-bis(1,1-dimethylethyl)-4-ethyl-
PvB43	4378-61-4	dibenzo[def,mno]chrysene-6,12-dione, 4,10-dibromo-
PvB46	512-04-9	spirost-5-en-3-ol, (3beta,25R)-
PvB47	51630-58-1	benzeneacetic acid, 4-chloro-alpha-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester
PvB48	5165-81-1	2-naphthalenecarboxamide, N-(4-chloro-2-methoxy-5-methylphenyl)-3-hydroxy-
PvB49	52434-90-9	1,3,5-triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris(2,3-dibromopropyl)-

Code no	CAS	Name
PvB51	5285-60-9	benzenamine, 4,4′-methylenebis[N-(1-methylpropyl)-
PvB59	732-26-3	phenol, 2,4,6-tris(1,1-dimethylethyl)-
PvB62	85-22-3	benzene, pentabromoethyl-
PvB64	90-93-7	methanone, bis[4-(diethylamino)phenyl]-
PvB65	93-46-9	1,4-benzenediamine, N,N′-di-2-naphthalenyl-
PvB66	128-70-1	8,16-pyranthrenedione
PvB68	13121-70-5	stannane, tricyclohexylhydroxy-
PvB69	13356-08-6	distannoxane, hexakis(2-methyl-2-phenylpropyl)-
PvB71	2223-93-0	octadecanoic acid, cadmium salt
PvB72	309-00-2	1,4:5,8-dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1.alpha.,4.alpha.,4a.beta.,5.alpha.,8.alpha.,8a.beta.)-
PvB75	3861-47-0	octanoic acid, 4-cyano-2,6-diiodophenyl ester
PvB76	40487-42-1	benzenamine, N-(1-ethylpropyl)-3,4-dimethyl-2,6-dinitro-
PvB77	41083-11-8	1H-1,2,4-triazole, 1-(tricyclohexylstannyl)-
PvB78	52315-07-8	cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester (cypermethrin)
PvB79	52645-53-1	cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, (3-phenoxyphenyl)methyl ester
PvB80	61951-96-0	neodecanoic acid, cadmium salt
PvB81	67375-30-8	cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester (alpha-cypermethrin)
PvB86	1861-40-1	benzenamine, N-butyl-N-ethyl-2,6-dinitro-4-(trifluoromethyl)-
PvB87	4051-63-2	[1,1′-bianthracene]-9,9′,10,10′-tetrone, 4,4′-diamino-
PvB90	19774-82-4	methanone, (2-butyl-3-benzofuranyl)[4-[2-(diethylamino)ethoxy]-3,5-diiodophenyl]-, hydrochloride
PvB92	36861-47-9	bicyclo(2.2.1)heptan-2-one, 1,7,7-trimethyl-3-[(4-methylphenyl)methylene]-
PvB96	68085-85-8	cyclopropanecarboxylic acid, 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester
PvB99	12239-34-8	acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-ethoxyphenyl]-
PvB100	1229-55-6	2-naphthalenol, 1-[(2-methoxyphenyl)azo]-
PvB101	14295-43-3	benzo[b]thiophen-3(2H)-one, 4,7-dichloro-2-(4,7-dichloro-3-oxobenzo[b]thien-2(3H)-ylidene)-
PvB102	15086-94-9	spiro[isobenzofuran-1(3H),9′-[9H]xanthen]-3-one, 2′,4′,5′,7′-tetrabromo-3′,6′-dihydroxy-
PvB103	15958-61-9	9,10-anthracenedione, 1-[[4-(phenylsulfonyl)phenyl]amino]-
PvB105	19800-42-1	phenol, 4-[[2-methoxy-4-[(4-nitrophenyl)azo]phenyl]azo]-
PvB106	20241-76-3	9,10-anthracenedione, 1,8-dihydroxy-4-nitro-5-(phenylamino)-
PvB107	23355-64-8	ethanol, 2,2′-[[3-chloro-4-[(2,6-dichloro-4-nitrophenyl)azo]phenyl]imino]bis-
PvB109	24610-00-2	benzonitrile, 2-[[4-[(2-cyanoethyl)(2-phenylethyl)amino]phenyl]azo]-5-nitro-
PvB111	2814-77-9	2-naphthalenol, 1-[(2-chloro-4-nitrophenyl)azo]-

Code no	CAS	Name
PvB112	3468-63-1	2-naphthalenol, 1-[(2,4-dinitrophenyl)azo]-
PvB115	475-71-8	benzo[h]benz[5,6]acridino[2,1,9,8-klmna]acridine-8,16-dione
PvB116	509-34-2	spiro[isobenzofuran-1(3H),9′-[9H]xanthen]-3-one, 3′,6′-bis(diethylamino)-
PvB117	5261-31-4	propanenitrile, 3-[[2-(acetyloxy)ethyl][4-[(2,6-dichloro-4-nitrophenyl)azo]phenyl]amino]-
PvB118	52697-38-8	acetamide, N-[2-[(2-bromo-4,6-dinitrophenyl)azo]-5-(diethylamino)phenyl]-
PvB121	59487-23-9	2-naphthalenecarboxamide, 4-[[5-[[[4-(aminocarbonyl)phenyl]amino]carbonyl]-2-methoxyphenyl]azo]-N-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxy-
PvB124	6250-23-3	phenol, 4-[[4-(phenylazo)phenyl]azo]-
PvB125	6407-78-9	3H-pyrazol-3-one, 4-[(2,4-dimethylphenyl)azo]-2,4-dihydro-5-methyl-2-phenyl-
PvB126	6410-41-9	2-naphthalenecarboxamide, N-(5-chloro-2,4-dimethoxyphenyl)-4-[[5-[(diethylamino)sulfonyl]-2-methoxyphenyl]azo]-3-hydroxy-
PvB127	64338-16-5	7-oxa-3,20-diazadispiro[5.1.11.2]heneicosan-21-one, 2,2,4,4-tetramethyl-
PvB128	65140-91-2	phosphonic acid, [[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-, monoethyl ester, calcium salt (2:1)
PvB130	6786-83-0	1-naphthalenemethanol, α,α-bis[4-(dimethylamino)phenyl]-4-(phenylamino)-
PvB133	70331-94-1	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, (1,2-dioxo-1,2-ethanediyl)bis(imino-2,1-ethanediyl) ester
PvB141	85-86-9	2-naphthalenol, 1-[[4-(phenylazo)phenyl]azo]-
PvB142	842-07-9	2-naphthalenol, 1-(phenylazo)-
PvB145	28219-61-6	2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol
PvB146	28371-99-5	methyl-2,6,10-trimethylcyclododeca-2,5,9-trien-1-yl ketone
PvB147	13171-00-1	6-tert-butyl-1,1-dimethylindan-4-yl methyl ketone
PvB148	87-44-5	caryophyllene
PvB149	65113-99-7	a,b,2,2,3-pentamethylcyclopent-3-ene-1-butanol
PvB150	77-54-3	[3R-(3a,3ab,6a,7b,8aa)]-octahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl acetate
PvB154	26040-51-7	phthalic acid, tetrabromo-, bis(2-ethylhexyl) ester
PvB155	58965-66-5	tetradecabromodiphenoxybenzene
PvB156	118-56-9	homosalate
PvB157	21245-02-3	ethylhexyl dimethyl dimethyl-*p*-aminobenzoate [ethylhexyl dimethyl PABA]
PvB158	6197-30-4	octocrylene
PvB159	15087-24-8	3-benzylidene camphor
PB11	467-63-0	benzenemethanol, 4-(dimethylamino)-alpha,alpha-bis[4-(dimethylamino)phenyl]-
PB12	50-65-7	benzamide, 5-chloro-N-(2-chloro-4-nitrophenyl)-2-hydroxy-
PB13	51-03-6	1,3-benzodioxole, 5-[[2-(2-butoxyethoxy)ethoxy]methyl]-6-propyl-
PB14	57018-04-9	phosphorothioic acid, O-(2,6-dichloro-4-methylphenyl) O,O-dimethyl ester
PB16	634-66-2	benzene, 1,2,3,4-tetrachloro-

Code no	CAS	Name
PB18	66063-05-6	urea, N-[(4-chlorophenyl)methyl]-N-cyclopentyl-N′-phenyl-
PB22	92-72-8	2-naphthalenecarboxamide, N-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxy-
PB23	101-20-2	urea, N-(4-chlorophenyl)-N′-(3,4-dichlorophenyl)-
PB25	41198-08-7	profenofos
PB26	50-63-5	1,4-pentanediamine, N(4)-(7-chloro-4-quinolinyl)-N(1),N(1)-diethyl-, phosphate (1:2)
PB27	116-29-0	benzene, 1,2,4-trichloro-5-[(4-chlorophenyl)sulfonyl]-
PB29	68015-60-1	benzenesulfonic acid, 2-amino-, (1-methylethylidene)di-4,1-phenylene ester
PB30	1937-37-7	2,7-naphthalenedisulfonic acid, 4-amino-3-[[4′-[(2,4-diaminophenyl)azo][1,1′-biphenyl]-4-yl]azo]-5-hydroxy-6-(phenylazo)-, disodium salt
PB32	56-95-1	2,4,11,13-tetraazatetradecanediimidamide, N,N″-bis(4-chlorophenyl)-3,12-diimino-, diacetate
PB34	81-68-5	benzenesulfonamide, N-(4-amino-9,10-dihydro-3-methoxy-9,10-dioxo-1-anthracenyl)-4-methyl-

Table 4.2 Medium-priority substances.

Code no	CAS	Name
PvB4	112-29-8	decane, 1-bromo-
PvB7	129-73-7	benzenamine, 4,4′-(phenylmethylene)bis[N,N-dimethyl-
PvB8	13393-93-6	1-phenanthrenemethanol, tetradecahydro-1,4a-dimethyl-7-(1-methylethyl)-
PvB9	135-91-1	benzenamine, 4,4′-methylenebis[N,N-diethyl-
PvB10	13680-35-8	benzenamine, 4,4′-methylenebis[2,6-diethyl-
PvB18	19941-28-7	1-phenanthrenecarboxylic acid, tetradecahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1alpha,4abeta,4balpha,7beta,8abeta,10aalpha)]-
PvB32	355-43-1	hexane, 1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-6-iodo-
PvB34	3739-67-1	benzene, 1,1′-(1-methylethylidene)bis[4-(2-propenyloxy)-
PvB36	38521-51-6	benzene, pentabromo(bromomethyl)-
PvB38	40567-16-6	butanoyl chloride, 2-[2,4-bis(1,1-dimethylpropyl)phenoxy]-
PvB41	42074-68-0	benzene, 1-chloro-2-(chlorodiphenylmethyl)-
PvB42	423-50-7	1-hexanesulfonyl fluoride, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-
PvB45	50772-29-7	butanoyl chloride, 4-[2,4-bis(1,1-dimethylpropyl)phenoxy]-
PvB50	52740-90-6	2-anthracenecarboxamide, 1-amino-N-(3-bromo-9,10-dihydro-9,10-dioxo-2-anthracenyl)-9,10-dihydro-9,10-dioxo-
PvB52	54079-53-7	propanedinitrile, [[4-[[2-(4-cyclohexylphenoxy)ethyl]ethylamino]-2-methylphenyl]methylene]-
PvB53	54914-37-3	cyclohexanemethanamine, 1,3,3-trimethyl-N-(2-methylpropylidene)-5-[(2-methylpropylidene)amino]-

Code no	CAS	Name
PvB54	55525-54-7	urea, N,N′-bis[(5-isocyanato-1,3,3-trimethylcyclohexyl)methyl]-
PvB55	56358-17-9	2-naphthalenamine, N-(2-ethylhexyl)-
PvB56	59447-55-1	2-propenoic acid, (pentabromophenyl)methyl ester
PvB57	63059-55-2	hexanoyl chloride, 2-[2,4-bis(1,1-dimethylpropyl)phenoxy]-
PvB58	63216-89-7	1H-indene-1,3(2H)-dione, 2-benzo[f]quinolin-3-yl-
PvB61	850-92-0	1,3-cyclopentanedione, 2-[2-(3,4-dihydro-6-methoxy-1(2H)-naphthalenylidene)ethyl]-2-ethyl-
PvB67	135-65-9	2-naphthalenecarboxamide, 3-hydroxy-N-(3-nitrophenyl)-
PvB70	15696-43-2	octanoic acid, lead salt
PvB73	3091-32-5	stannane, chlorotricyclohexyl-
PvB82	81-98-1	7H-benz[de]anthracen-7-one, 3,9-dibromo-
PvB83	128-83-6	perylo[3,4-cd:9,10-c′d′]dipyran-1,3,8,10-tetrone
PvB84	375-72-4	1-butanesulfonyl fluoride, 1,1,2,2,3,3,4,4,4-nonafluoro-
PvB88	7139-02-8	pyrimido[5,4-d]pyrimidine, 2,6-dichloro-4,8-di-1-piperidinyl-
PvB89	15114-15-5	9,10-anthracenedione, 4,8-diamino-2-(4-ethoxyphenyl)-1,5-dihydroxy-
PvB93	38521-51-6	benzene, pentabromo(bromomethyl)-
PvB95	41999-84-2	benzene, 1,4-dichloro-2,5-bis(dichloromethyl)-
PvB97	1068-27-5	peroxide, (1,1,4,4-tetramethyl-2-butyne-1,4-diyl)bis[(1,1-dimethylethyl)
PvB98	12236-64-5	2-naphthalenecarboxamide, N-[4-(acetylamino)phenyl]-4-[[5-(aminocarbonyl)-2-chlorophenyl]azo]-3-hydroxy-
PvB104	17464-91-4	ethanol, 2,2′-[[4-[(2-bromo-6-chloro-4-nitrophenyl)azo]-3-chlorophenyl]imino]bis-
PvB110	25155-25-3	peroxide, [1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[(1,1-dimethylethyl)
PvB113	42739-61-7	nickel, bis[2,3-bis(hydroxyimino)-N-(2-methoxyphenyl)butanamidato]-
PvB114	43035-18-3	benzenesulfonic acid, 4-[[3-[[2-hydroxy-3-[[(4-methoxyphenyl)amino]carbonyl]-1-naphthalenyl]azo]-4-methylbenzoyl]amino]-, calcium salt (2:1)
PvB119	53184-75-1	phosphorous acid, (1-methylethylidene)di-4,1-phenylene tetrakis[(3-ethyl-3-oxetanyl)methyl] ester
PvB122	59709-10-3	pyridinium, 1-[2-[[4-[(2-chloro-4-nitrophenyl)azo]phenyl]ethylamino]ethyl]-, acetate
PvB123	59709-38-5	β-alanine, N-[4-[(2-bromo-6-chloro-4-nitrophenyl)azo]phenyl]-N-(3-methoxy-3-oxopropyl)-, methyl ester
PvB129	6731-36-8	peroxide, (3,3,5-trimethylcyclohexylidene)bis[(1,1-dimethylethyl)
PvB131	68391-08-2	alcohols, C8–14, γ-ω-perfluoro
PvB132	68877-63-4	acetamide, N-[2-[(2-bromo-4,6-dinitrophenyl)azo]-5-[(2-cyanoethyl)-2-propenylamino]-4-methoxyphenyl]-
PvB134	70660-55-8	1-naphthalenamine, 4-[(2-bromo-4,6-dinitrophenyl)azo]-N-(3-methoxypropyl)-
PvB135	72869-85-3	chromate(1-), bis[3,5-bis(1,1-dimethylethyl)-2-hydroxybenzoato(2-)-O1,O2]-, hydrogen
PvB136	72968-82-2	methanesulfonamide, N-[2-[(2,6-dicyano-4-methylphenyl)azo]-5-(dipropylamino)phenyl]-
PvB137	74336-60-0	9,10-anthracenedione, 1-[(5,7-dichloro-1,9-dihydro-2-methyl-9-oxopyrazolo[5,1-b]quinazolin-3-yl)azo]-

Code no	CAS	Name
PvB138	78-63-7	peroxide, (1,1,4,4-tetramethyl-1,4-butanediyl)bis[(1,1-dimethylethyl)
PvB139	83006-67-1	benzenesulfonic acid, 2,2′-[(9,10-dihydro-5,8-dihydroxy-9,10-dioxo-1,4-anthracenediyl)diimino]bis[5-(1,1-dimethylethyl)-, disodium salt
PvB140	85702-64-3	3H-indol-3-one, 5,7-dibromo-2-(5-bromo-7-chloro-1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-
PvB153	25327-89-3	tetrabromobisphenol-A bis(allylether)
PB1	10310-32-4	D-glucofuranoside, ethyl 3,5,6-tris-O-(phenylmethyl)-
PB2	119-94-8	benzenemethanamine, N-ethyl-N-(3-methylphenyl)-
PB4	133-91-5	benzoic acid, 2-hydroxy-3,5-diiodo-
PB5	15307-93-4	benzenamine, 2,6-dichloro-N-phenyl-
PB7	41604-19-7	1,1′-biphenyl, 4-bromo-2-fluoro-
PB8	4273-92-1	2-naphthalenecarboxamide, N-(4-chloro-2,5-dimethoxyphenyl)-3-hydroxy-
PB9	43076-61-5	1-butanone, 4-chloro-1-[4-(1,1-dimethylethyl)phenyl]-
PB10	464-41-5	bicyclo[2.2.1]heptane, 2-chloro-1,7,7-trimethyl-, endo-
PB15	626-39-1	benzene, 1,3,5-tribromo-
PB17	63734-62-3	benzoic acid, 3-[2-chloro-4-(trifluoromethyl)phenoxy]-
PB19	7785-70-8	bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-, (1R)-
PB28	52179-28-9	propanoic acid, 2-[4-(2,2-dichlorocyclopropyl)phenoxy]-2-methyl-, ethyl ester
PB31	2778-42-9	benzene, 1,3-bis(1-isocyanato-1-methylethyl)-
PB33	72828-93-4	1-propanaminium, 3-[[9,10-dihydro-4-[(4-methylphenyl)amino]-9,10-dioxo-1-anthracenyl]amino]-N,N,N-trimethyl-, methyl sulfate

Table 4.3 Low-priority substances.

Code no	CAS	Name
PvB2	104-42-7	benzenamine, 4-dodecyl-
PvB40	4162-45-2	ethanol, 2,2′-[(1-methylethylidene)bis[(2,6-dibromo-4,1-phenylene)oxy]]bis-
PvB63	87-83-2	benzene, pentabromomethyl-
PvB85	632-79-1	1,3-isobenzofurandione, 4,5,6,7-tetrabromo-
PvB91	21850-44-2	benzene, 1,1′-(1-methylethylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)-
PvB108	2425-85-6	2-naphthalenol, 1-[(4-methyl-2-nitrophenyl)azo]-
PvB143	67-97-0	colecalciferol, Vitamin D3

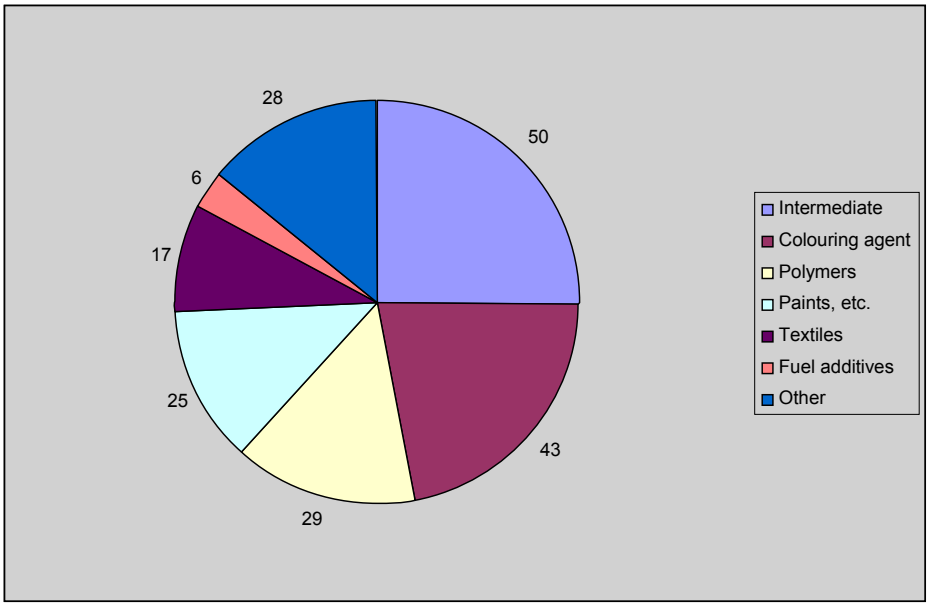
Code no	CAS	Name
PvB144	21145-77-7	1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthyl)ethan-1-one
PvB151	96-69-5	4,4′-thio-bis(2-t-butyl-5-methylphenol)[23]
PvB152	13560-89-9	dodecachlorodimethan-o-dibenzocyclooctane[20]
PB3	129-00-0	pyrene
PB6	3380-34-5	phenol, 5-chloro-2-(2,4-dichlorophenoxy)-
PB20	82-05-3	7H-benz[de]anthracen-7-one
PB35	1335-46-2	ionone, methyl -
PB36	127-51-5	3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one

[23] This substance had been considered by the European Commission PBT Working Group previously, but a decision was deferred.

4.2 Use pattern assessment

The use pattern information obtained during this project comes from the IUCLID 4 database and other sources. The IUCLID 4 information is confidential, and so cannot be included in detail here. It consists of 'use categories' assigned to the substances by the registrants according to the Technical Guidance Document for the ESR.[24] A summary of the information from this source is presented in Figure 4.1 (for the 184 substances considered after the initial screen). Note that some substances are allocated to more than one use type, and so the total number of uses is greater than the number of substances. There are 11 use categories represented in the 'Other' group in the figure.

Figure 4.1 Distribution of use categories from IUCLID 4 data.



The use information from other sources is included in the fact sheets for each substance (Appendix 2). For 75 of the substances, no non-confidential information was located. The uses for the remaining 109 substances are compiled in Table 4.4 (two substances have two uses).

24 http://ecb.jrc.ec.europa.eu/documents/TECHNICAL_GUIDANCE_DOCUMENT/EDITION_2/tgdpart2_2ed.pdf

Table 4.4 Use-pattern information from public sources.

Use (number of substances)	Substances (by code number)
Dye/pigment (27)	PvB: 43, 48, 66, 99, 100, 101, 102, 105, 106, 108, 111, 115, 116, 117, 118, 121, 124, 125, 126, 127, 130, 141, 142
	PB: 11, 22, 30, 34
Plant protection product (17)	PvB: 47, 68, 69, 72, 75, 76, 77, 78, 79, 81, 86, 96
	PB: 13, 14, 18, 25, 27
Fire retardant (15)	PvB: 1, 17, 28, 40, 49, 56, 63, 85, 91, 93, 151, 152, 153, 154, 155
Fragrance (12)	PvB: 3, 26, 30, 144, 145, 146, 147, 148, 149, 150
	PB: 35, 36
UV stabiliser (10)	PvB: 25, 33, 37, 71, 92, 127, 156, 157, 158, 159
Intermediate (9)	PvB: 41, 67, 82, 131
	PB: 1, 8, 16, 19, 20
Anti-oxidant/ozonant (5)	PvB: 11, 13, 39, 128, 133
Polymer cross-linker (5)	PvB: 97, 110, 129, 138
	PB: 31
Biocide (3)	PB: 6, 23, 26
Drug (3)	PvB: 19, 46
	PB: 26
Animal medicine (1)	PB: 12
Coatings (1)	PvB: 21
Electronics (1)	PvB: 31
Fabric brightener (1)	PvB: 27
Food additive (1)	PvB: 143

The two sets of information do have some differences, which we have not investigated in depth for this project. The use category information in IUCLID does not always go into the same detail as found in other sources; for example, substances described as fire retardants in Table 4.4 may have been described only as ‘used in polymers’ in IUCLID. Also, a large number of the substances for which no public information on uses was located are described as synthetic intermediates in IUCLID.

Some of the identified uses are not subject to the REACH Regulation – plant protection products, biocides, drugs, animal medicines and food additives – although if the substances have other minor uses these could be covered. It is likely that more data are available for most of the substances used in these applications.

The use of a substance can give an initial indication of the likelihood of release to the environment during the use stage of the life cycle, and an indication of this is included in each of the fact sheets. From Table 4.4, the uses most likely to lead to widespread release are as fragrances, plant protection products and biocides. The use areas with the least likelihood of release are as an intermediate or cross-linking agent in polymers. In the case of intermediate use, release is still possible if the product is capable of degrading and reforming the original substance. This is less likely with cross-linking agents. The other uses probably have an intermediate likelihood of significant release. In all cases the properties of the individual substances will have an influence on the possibility of release, and so this initial categorisation is rather crude. The nature of the material in which the substance is included (if that is part of the use) will also influence exposure potential; for example, an anti-oxidant used in cosmetic products may be more likely to reach the environment (through being washed off the body) than the same substance used for the same purpose in plastics.

4.3 Grouping by structural features

As mentioned in Section 1, the European Commission has already assessed HPV substances in detail for PBT properties, and fact sheets for over 125 substances are published.[25]

Although it is beyond the scope of this report to make a detailed comparison of these with the LPV substances, some observations can be made:

- Only a relatively small number of substances have been confirmed as meeting the Annex XIII criteria. These are summarised in Table 4.5. Some of these substances are considered to be of equivalent concern [for example, because of long-range transport potential or listing on the Stockholm Convention on Persistent Organic Pollutants (POPs) (http://chm.pops.int)].

Table 4.5 HPV substances that have confirmed PBT or vPvB properties (or are of equivalent concern).

CAS No.	Substance name
58-89-9	lindane
50-29-3	1,1,1-trichloro-2,2-bis(4-chlorophenyl)ethane (clofenotane or p,p-DDT)
56-35-9	bis(tributyltin) oxide (TBTO)
81-15-2	5-tert-butyl-2,4,6-trinitro-m-xylene)musk xylene)
87-61-6	1,2,3-trichlorobenzene
87-68-3	hexachlorobuta-1,3-diene
115-29-7	endosulfan
115-32-2	dicofol
118-74-1	hexachlorobenzene
120-12-7	anthracene, pure
120-82-1	1,2,4-trichlorobenzene
1836-75-5	nitrofen
25637-99-4	hexabromocyclododecane
32536-52-0	diphenyl ether, octabromo derivative (octabromodiphenyl ether)
65996-93-2	coal tar pitch, high temperature
85535-84-8	alkanes, $C_{10–13}$, chloro [short-chain chlorinated paraffins (SCCPs)]
90640-80-5	anthracene oil
90640-81-6	anthracene oil, anthracene paste
90640-82-7	anthracene oil, anthracene-low
90640-86-1	distillates (coal tar), heavy oils
91995-15-2	anthracene oil, anthracene paste, anthracene fraction
91995-17-4	anthracene oil, anthracene paste, distillation lights
91995-42-5	distillates (coal tar), heavy oils, pyrene fraction
91995-52-7	distillates (coal tar), pitch, pyrene fraction
92061-94-4	residues (coal tar), pitch distillation

[25] http://ecb.jrc.ec.europa.eu/home.php?CONTENU=/DOCUMENTS/PBT_EVALUATION/

The majority are either pesticides or contain polyaromatic hydrocarbons (PAHs) that are themselves considered to have PBT or vPvB properties. It is also notable that there is an organotin compound and some highly halogenated substances. The only other type of substance is 5-tert-butyl-2,4,6-trinitro-m-xylene (an artificial musk fragrance).

- Some additional substances are addressed by the Stockholm Convention or the United Nations Economic Commission for Europe Protocol on POPs[26], but have not been discussed as such by the PBT Working Group. These compounds are:
  - chlordane (CAS no. 57-74-9)
  - dieldrin (CAS no. 60-57-1)
  - endrin (CAS no. 72-20-8)
  - heptachlor (CAS no. 76-44-8)
  - chlordecone (kepone) (CAS no. 143-50-0)
  - aldrin (CAS no. 309-00-2)
  - pentachlorobenzene (CAS no. 608-93-5)
  - mirex (CAS no. 2385-85-5)
  - toxaphene (CAS no. 8001-35-2)
  - hexabromobiphenyl (CAS no. 36355-01-8)
  - polychlorinated biphenyls (PCBs)
  - polychlorinated dibenzo-*p*-dioxins and dibenzofurans (PCDD/PCDFs)
  - tetra- to heptabromodiphenyl ethers
  - perfluorooctane sulfonic acid, its salts and perfluorooctane sulfonyl fluoride.

  To this list might also be added certain substances that are already subject to restrictions in the EU, for example polychlorinated terphenyls and polybromobiphenyls. All of these substances are either pesticides or highly halogenated (mostly both).

  A decision for a more diverse group of substances is pending the receipt of further information, as indicated in Table 4.6.

26 http://www.unece.org/env/lrtap/pops_h1.htm

Table 4.6 HPV substances that are *potentially* PBT or vPvB (or of equivalent concern) and require further evaluation.

CAS No.	Substance name
75-74-1	tetramethyllead
77-47-4	hexachlorocyclopentadiene
118-82-1	2,2',6,6'-tetra-tert-butyl-4,4'-methylenediphenol
133-49-3	pentachlorobenzenethiol
294-62-2	cyclododecane
541-02-6	decamethylcyclopentasiloxane
556-67-2	octamethylcyclotetrasiloxane
608-71-9	pentabromophenol
1163-19-5	bis(pentabromophenyl) ether (decabromodiphenyl ether)
1461-25-2	tetrabutyltin
3542-36-7	dichlorodioctylstannane
3590-84-9	tetraoctyltin
15571-58-1	2-ethylhexyl-10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate
25103-58-6	tert-dodecanethiol
26140-60-3	terphenyl
27107-89-7	2-ethylhexyl-10-ethyl-4-[[2-[(2-ethylhexyl)oxy]-2-oxoethyl]-thio]-4-octyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate
31565-23-8	di(tert-dodecyl)pentasulfide
38640-62-9	di(isopropyl)naphthalene
39489-75-3	bis(2,4-dichloro-5-nitrophenyl)carbonate
50849-47-3	5-nonylsalicylaldehyde oxime
61788-32-7	terphenyl, hydrogenated
61788-44-1	phenol, styrenated
64742-04-7	extracts (petroleum) heavy paraffin distillate solvent
68442-68-2	benzenamine, N-phenyl-, styrenated
83846-43-9	benzoic acid, 2-hydroxy-, mono-$C_{>13}$-alkyl derivatives, calcium salts (2:1)
84929-98-6	magnesium, bis(2-hydroxybenzoato-O1,O2)-, ar,ar'-di-$C_{>13}$-alkyl derivatives
84852-14-2	2,4-dinonylphenol, branched
85535-85-9	alkanes, $C_{14–17}$, chloro [medium-chain chlorinated paraffins (MCCPs)]
90481-05-3	phenol, nonyl-, manufacture of, by-products from, high-boiling
91696-73-0	benzenesulfonic acid, $C_{14–44}$-branched and linear alkyl derivatives, calcium salts
91745-46-9	amines, $C_{12–14}$-alkyl, reaction products with hexanol, phosphorus oxide (P_2O_5), phosphorus sulfide (P_2S_5) and propylene oxide

Note: This table includes a small number of substances for which either a decision on further data requirements was not taken, or for which PBT properties were concluded on the basis of screening information only, because no suppliers were identified. For example, tetramethyllead (CAS no. 75-74-1) was concluded to be a PBT but is unlikely to be persistent, by analogy with tetraethyllead (CAS no. 78-00-2).

We have not carried out a full similarity analysis of the structures of the prioritised LPV substances, but a review of the listings by eye (and when compiling the fact sheets) identified a number of structural types that occur several times:

a) The largest group is benzenamines, including the following substances (by code number):

   PvB: 2, 7, 9, 10, 11, 13, 22, 23, 24, 51, 65, 76, 86; PB: 5

   These substances are used mainly as intermediates in synthesis. Two related substances[27] were reviewed by the EU PBT WG, and considered not to be persistent because of fast hydrolysis (and the degradation products are not bioaccumulative).

b) A second group is based on the benzotriazole structure. These are used mainly as UV stabilisers:

   PvB: 21, 25, 33, 35, 37

   This substance type does not appear to have been discussed by the PBT Working Group before.

c) Five phenylazo derivatives of 2-naphthalenol:

   PvB: 100, 111, 112, 141, 142

   Again, this substance type does not appear to have been discussed by the PBT Working Group before.

d) Three alkanoyl chlorides:

   PvB: 38, 45, 57

   Confidential use information indicates that these are used as reactants, and so they would be expected to have a relatively low exposure potential. It is also likely that these substances would hydrolyse or react with other substances in the environment. No current suppliers were located.

e) Three heavy metal salts of long-chain carboxylic acids are included in the high-priority group:

   PvB: 70, 71, 80

   The organic acid component of these is likely to be of lower concern, so these substances may also be of lower concern on further investigation.

f) Three highly substituted alkylphenols:

   PvB: 15, 39, 59

[27] N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6PPD), CAS no. 793-24-8; and 1,4,-benzenediamine, N,N'-mixed phenyl and tolyl derivatives, CAS no. 68953-84-4.

PvB: 70, 71, 80

The organic acid component of these is likely to be of lower concern, so these substances may also be of lower concern on further investigation.

f) Three highly substituted alkylphenols:

PvB: 15, 39, 59

Based on the crude analysis of confirmed PBT and vPvB substances carried out above, a further review of organotins, highly halogenated and PAH-like substances might be particularly useful. From the high-priority group, this includes:

PvB: 12, 29, 31, 43, 62, 66, 68, 69, 72, 77, 87, 101, 102, 115, 154, 155; PB: 16

However, as shown by musk xylene, other structural types should not be discounted from further consideration and all substances should be considered on their own merits.

5 Conclusions

Out of 7829 substances considered to be supplied to the European market by individual suppliers in the range 10-1000 tonnes/year, we identified 184 as candidates for further investigation, divided into three groups: 103 are high priority, 66 medium priority and 15 low priority. None of these is a confirmed PBT or vPvB substance at this stage.

Although all of the prioritised substances will need further evaluation, based on a crude analysis of confirmed PBT and vPvB substance structural types, a further review of organotins, highly halogenated and PAH-like substances might be particularly useful. Fragrances with a high potential for exposure should also be examined. Table 5.1 lists 26 relevant substances from the high-priority group.

Table 5.1 Substances that could be evaluated first.

Code no	CAS	Name
PvB3	11028-42-5	cedrene
PvB12	1484-08-8	9H-carbazole, 9-butyl-
PvB26	32388-55-9	ethanone, 1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)-, [3R-(3alpha,3abeta,7beta,8aalpha)]-
PvB29	335-57-9	heptane, hexadecafluoro-
PvB30	3407-42-9	cyclohexanol, 3-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)-
PvB31	355-42-0	hexane, tetradecafluoro-
PvB43	4378-61-4	dibenzo[def,mno]chrysene-6,12-dione, 4,10-dibromo-
PvB62	85-22-3	benzene, pentabromoethyl-
PvB66	128-70-1	8,16-pyranthrenedione
PvB68	13121-70-5	stannane, tricyclohexylhydroxy-
PvB69	13356-08-6	distannoxane, hexakis(2-methyl-2-phenylpropyl)-
PvB72	309-00-2	1,4:5,8-dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1.alpha.,4.alpha.,4a.beta.,5.alpha.,8.alpha.,8a.beta.)-
PvB77	41083-11-8	1H-1,2,4-triazole, 1-(tricyclohexylstannyl)-
PvB87	4051-63-2	(1,1′-bianthracene)-9,9′,10,10′-tetrone, 4,4′-diamino-
PvB101	14295-43-3	benzo[b]thiophen-3(2H)-one, 4,7-dichloro-2-(4,7-dichloro-3-oxobenzo[b]thien-2(3H)-ylidene)-
PvB102	15086-94-9	spiro[isobenzofuran-1(3H),9′-[9H]xanthen]-3-one, 2′,4′,5′,7′-tetrabromo-3′,6′-dihydroxy-
PvB115	475-71-8	benzo[h]benz[5,6]acridino[2,1,9,8-klmna]acridine-8,16-dione
PvB145	28219-61-6	2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol
PvB146	28371-99-5	methyl 2,6,10-trimethylcyclododeca-2,5,9-trien-1-yl ketone
PvB147	13171-00-1	6-tert-butyl-1,1-dimethylindan-4-yl methyl ketone
PvB148	87-44-5	caryophyllene
PvB149	65113-99-7	a,b,2,2,3-pentamethylcyclopent-3-ene-1-butanol
PvB150	77-54-3	[3R-(3a,3ab,6a,7b,8aa)]-octahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl acetate
PvB154	26040-51-7	phthalic acid, tetrabromo-, bis(2-ethylhexyl) ester
PvB155	58965-66-5	tetradecabromodiphenoxybenzene
PB16	634-66-2	benzene, 1,2,3,4-tetrachloro-

This study has resulted in changes to the findings from previous reviews in some cases. Five substances identified as potential PBTs in Environment Agency (2003) are now considered not to meet the criteria based on experimental data identified for this project. As noted in Section 3.1, we conducted only a brief search for such data, and therefore further changes are expected from a more detailed investigation. Also, we used the experimental results 'as found', and so a reduction in priority based on these results should be considered *provisional* pending a more detailed check of the data set.

The screen is related to PBT properties. For the purposes of this review we limited the consideration of CMR substances to those on the LPV list. R48 substances were considered on the same basis.

We could not identify potential vPvB substances, as screening criteria to distinguish between P and vP have not been developed and the available predictive methods for degradation do not provide results comparable to the actual vP criteria. It is also questionable whether a screening exercise based solely on estimated fate data is of value in this context.

We stress that we have not scrutinised the raw data in any detail and, in particular, the report relies on a single QSAR program (EPI SUITE^{TM}). Any QSAR method should be used cautiously, and a detailed substance evaluation needs to assess the appropriateness of the technique in comparison with other models. However, this project is a simple sifting exercise to identify candidates for more in-depth evaluation. Further evaluation will take time, and will need to consider measured data available within chemical companies as well as other QSAR methods, analogue read-across, etc., in a weight-of-evidence assessment. Further assessment could therefore lead to a change in the priority of any of these substances (whether through use pattern or properties – for example, only aquatic biodegradation has was assessed for this report, but several substances could be expected to degrade abiotically at a relatively fast rate). There is also a risk that the approach adopted for this report might have missed some substances. Since industry has the responsibility of compiling and justifying data sets under REACH, and to perform their own PBT assessments as part of their registration requirements, we recommend this report be revisited after the appropriate registration deadline has passed (the first of these is 1 December 2010).

Consequently, the output of this report should be viewed as a working list with no legal standing, and it must not be taken to imply that an Annex XV dossier will be brought forward for any individual substance that has currently been identified as a high or medium priority for further work. Instead, it is a contribution to further priority-setting activities by regulatory authorities in the UK and elsewhere in Europe, and for industry as they prepare for registration and test plan development under REACH.

The report does not consider inorganic substances, complex substances for which no discrete structure can be identified, or substances for which CAS numbers were not included in the EPI SUITE^{TM} database (see Appendix 4). They could be reviewed if REACH registrations are submitted in the future. Degradation products that are not supplied as such are also excluded. Other substances (for example, those that cause toxicity by interfering with endocrine systems) may also be priorities in the future, but we did not consider such properties in this review.

Abbreviations

BCF	Bioconcentration factor
BMF	Biomagnification factor
CAS	Chemical Abstracts Service
ChV	Chronic value; predicted by some equations in EPI SUITE^{TM}, and equivalent to the geometric mean of the NOEC and LOEC
CMR	Carcinogenic, mutagenic, reprotoxic
DOC	Dissolved organic carbon
DSL	Domestic Substance List
ECB	European Chemicals Bureau
EPA	Environment Protection Agency
ESIS	European Chemical Substances Information System
EINECS	European Inventory of Existing Commercial Chemical Substances
HPV	High production volume
HSE	Health and Safety Executive
IUCLID	International Uniform Chemical Information Database
K_{ow}	*n*-Octanol–water partition coefficient
L(E)C_{50}	The concentration that produces 50 per cent lethality of effect
LOEC	Lowest observed effect concentration
LPV	Low production volume
M-CASE	Multiple computer automated structure evaluation
NOEC	No observed effect concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, bioaccumulative and toxic
PBiT	Persistent, bioaccumulative and inherently toxic to non-human organisms
PBiThuman	Persistent, bioaccumulative and inherently toxic to humans
QSAR	Quantitative structure–activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
R48	Classification indicating danger of serious damage to health by prolonged exposure
R50	Classification for a substance with an LC_{50} less than 1 mg/l
R51	Classification for a substance with an LC_{50} between 1 mg/l and 10 mg/l
R52	Classification for a substance with an LC_{50} between 10 mg/l and 100 mg/l
R53	Classification indicating that a substance may cause long-term adverse effects in the aquatic environment
UKCSF	UK Chemicals Stakeholder Forum
vPvB	Very persistent and very bioaccumulative

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Appendix 1 CSF prioritisation criteria

A1.1 Key prioritisation criteria

A1.1.1 PBT, vPvB and CMR substances. Substances that meet the REACH Annex XIII criteria (PBT and vPvB) or categories 1 and 2 carcinogens, mutagens and reproductive toxins should be given equally high priority for authorisation; within these, substances for which no threshold effects could be demonstrated and/or there is evidence additive effects are likely should be given the highest priority.

A1.1.2 Pattern of use. Substances prioritised according to A1.1.1 and with known dispersive uses (even if not in the UK) should be considered of greater priority, since they are more likely to lead to exposure. Substances with closed uses only would be of lower concern.

A1.1.3 Equivalent concern. The UKCSF reserved the right to prioritise substances of equivalent concern, where they were likely to have an impact on human health and/or the environment.

A1.2 Criteria for refinement of the substance prioritisation

A1.2.1 Properties based on measurement or modelling data. Modelling data would usually represent the worst-case scenario and so substances for which the properties have been confirmed by available data should take greater priority. **Note:** if there is indication that a substance might meet the PBT, vPvB and/or CMR criteria but has insufficient data for completion of an Annex XV dossier for nomination of substances of highest concern, the UKCSF should consider that the missing data will be submitted with the Registration Dossier, and so it may be more appropriate to prioritise such a substance for evaluation.

A1.2.2 Production volume. The production volume would not be very informative; however ,it should be considered for prioritisation of substances with significant dispersive uses.

A1.2.3 Monitoring data. Monitoring data would be available for a limited number of substances, however greater priority should be given to substances if there are data in the UK or other countries that caused concern (for example, evidence that concentrations in the environment are increasing, or already high, or there is evidence of long-distance transport).

A1.2.4 Availability of alternatives. The availability of alternatives for relevant applications could be a factor.

A1.3. Further considerations

The prioritisation of substances for authorisation should give consideration to using a group approach for substances that are chemically and/or toxicologically related and/or likely to have additive effects on human health and the environment.

Appendix 2 Fact sheets

This appendix contains the fact sheets for the substances identified as possible substances of very high concern in this study. The sheets are arranged in order of the project code number assigned in this study, PvB substances first and then PB substances. To help locate substances, the appendix includes lists of PvB and PB substances in CAS number order. The lists also include the original source of the substance in terms of the existing study or exercise, as described in Section 2.2.

The sources of information in the fact sheets are indicated as far as possible (EA = Environment Agency). Predicted values generated for this study are indicated as EPI SUITE™ (for physicochemical and fate properties[28]) or ECOSAR™ (for aquatic toxicity). Measured values come from the sources listed in Section 3, and use-pattern information is indicated as coming from either *Kirk-Othmer* or from the web searches. The source of the original identification as 'T' (the original classification and/or screening exercise) is also indicated in the Ecotoxicity comments in the fact sheets.

[28] Different models were used for the various properties. For example, water solubility was estimated from the predicted log K_{ow} using the WSKOWWIN program in EPI SUITE.

Table A2.1 PvB substances ordered by CAS number.

Code number	Source	CAS	Substance
PvB1	D(a)	10192-93-5	benzene, 1,1′-(1,2-diethyl-1,2-dimethyl-1,2-ethanediyl)bis-
PvB2	D(a)	104-42-7	benzenamine, 4-dodecyl-
PvB97	DSL-E	1068-27-5	peroxide, (1,1,4,4-tetramethyl-2-butyne-1,4-diyl)bis[(1,1-dimethylethyl)
PvB3	D(a)	11028-42-5	cedrene
PvB4	D(a)	112-29-8	decane, 1-bromo-
PvB156	UV	118-56-9	homosalate
PvB98	DSL-E	12236-64-5	2-naphthalenecarboxamide, N-[4-(acetylamino)phenyl]-4-[[5-(aminocarbonyl)-2-chlorophenyl]azo]-3-hydroxy-
PvB99	DSL-E	12239-34-8	acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-ethoxyphenyl]-
PvB100	DSL-E	1229-55-6	2-naphthalenol, 1-[(2-methoxyphenyl)azo]-
PvB66	D(b)	128-70-1	8,16-pyranthrenedione
PvB83	O	128-83-6	perylo[3,4-cd:9,10-c′d′]dipyran-1,3,8,10-tetrone
PvB7	D(a)	129-73-7	benzenamine, 4,4′-(phenylmethylene)bis[N,N-dimethyl-
PvB68	N	13121-70-5	stannane, tricyclohexylhydroxy-
PvB147	F	13171-00-1	6-tert-butyl-1,1-dimethylindan-4-yl methyl ketone
PvB69	N	13356-08-6	distannoxane, hexakis(2-methyl-2-phenylpropyl)-
PvB8	D(a)	13393-93-6	1-phenanthrenemethanol, tetradecahydro-1,4a-dimethyl-7-(1-methylethyl)-
PvB152	FR	13560-89-9	dodecachlorodimethan-o-dibenzocyclooctane
PvB67	D(b)	135-65-9	2-naphthalenecarboxamide, 3-hydroxy-N-(3-nitrophenyl)-
PvB9	D(a)	135-91-1	benzenamine, 4,4′-methylenebis[N,N-diethyl-
PvB10	D(a)	13680-35-8	benzenamine, 4,4′-methylenebis[2,6-diethyl-
PvB11	D(a)	139-60-6	1,4-benzenediamine, N,N′-bis(1-ethyl-3-methylpentyl)-
PvB101	DSL-E	14295-43-3	benzo[b]thiophen-3(2H)-one, 4,7-dichloro-2-(4,7-dichloro-3-oxobenzo[b]thien-2(3H)-ylidene)-
PvB12	D(a)	1484-08-8	9H-carbazole, 9-butyl-
PvB102	DSL-E	15086-94-9	spiro[isobenzofuran-1(3H),9′-[9H]xanthen]-3-one, 2′,4′,5′,7′-tetrabromo-3′,6′-dihydroxy-
PvB159	UV	15087-24-8	3-benzylidene camphor
PvB89	O	15114-15-5	9,10-anthracenedione, 4,8-diamino-2-(4-ethoxyphenyl)-1,5-dihydroxy-
PvB13	D(a)	15233-47-3	1,4-benzenediamine, N-(1-methylheptyl)-N′-phenyl-
PvB70	N	15696-43-2	octanoic acid, lead salt
PvB103	DSL-E	15958-61-9	9,10-anthracenedione, 1-[[4-(phenylsulfonyl)phenyl]amino]-
PvB104	DSL-E	17464-91-4	ethanol, 2,2′-[[4-[(2-bromo-6-chloro-4-nitrophenyl)azo]-3-chlorophenyl]imino]bis-
PvB15	D(a)	17540-75-9	phenol, 2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-
PvB86	O	1861-40-1	benzenamine, N-butyl-N-ethyl-2,6-dinitro-4-(trifluoromethyl)-
PvB17	D(a)	1889-67-4	benzene, 1,1′-(1,1,2,2-tetramethyl-1,2-ethanediyl)bis-

Code number	Source	CAS	Substance
PvB90	O	19774-82-4	methanone, (2-butyl-3-benzofuranyl)[4-[2-(diethylamino)ethoxy]-3,5-diiodophenyl]-, hydrochloride
PvB105	DSL-E	19800-42-1	phenol, 4-[[2-methoxy-4-[(4-nitrophenyl)azo]phenyl]azo]-
PvB18	D(a)	19941-28-7	1-phenanthrenecarboxylic acid, tetradecahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1alpha,4abeta,4balpha,7beta,8abeta,10aalpha)]-
PvB106	DSL-E	20241-76-3	9,10-anthracenedione, 1,8-dihydroxy-4-nitro-5-(phenylamino)-
PvB144	F	21145-77-7	1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthyl)ethan-1-one
PvB157	UV	21245-02-3	ethylhexyl dimethyl PABA
PvB91	O	21850-44-2	benzene, 1,1′-(1-methylethylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)-
PvB71	N	2223-93-0	octadecanoic acid, cadmium salt
PvB107	DSL-E	23355-64-8	ethanol, 2,2′-[[3-chloro-4-[(2,6-dichloro-4-nitrophenyl)azo]phenyl]imino]bis-
PvB19	D(a)	23593-75-1	1H-imidazole, 1-[(2-chlorophenyl)diphenylmethyl]-
PvB20	D(a)	2422-91-5	benzene, 1,1′,1″-methylidynetris[4-isocyanato-
PvB108	DSL-E	2425-85-6	2-naphthalenol, 1-[(4-methyl-2-nitrophenyl)azo]-
PvB109	DSL-E	24610-00-2	benzonitrile, 2-[[4-[(2-cyanoethyl)(2-phenylethyl)amino]phenyl]azo]-5-nitro-
PvB110	DSL-E	25155-25-3	peroxide, [1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[(1,1-dimethylethyl)
PvB153	FR	25327-89-3	tetrabromobisphenol-A bis(allylether)
PvB21	D(a)	25973-55-1	phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)-
PvB154	FR	26040-51-7	phthalic acid, tetrabromo-, bis(2-ethylhexyl) ester
PvB111	DSL-E	2814-77-9	2-naphthalenol, 1-[(2-chloro-4-nitrophenyl)azo]-
PvB145	F	28219-61-6	2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol
PvB146	F	28371-99-5	methyl 2,6,10-trimethylcyclododeca-2,5,9-trien-1-yl ketone
PvB22	D(a)	29312-59-2	benzenamine, 4-(2,6-diphenyl-4-pyridinyl)-N,N-dimethyl-
PvB23	D(a)	29398-96-7	[1,1′-biphenyl]-4,4′-diamine, N,N′-bis(2,4-dinitrophenyl)-3,3′-dimethoxy-
PvB24	D(a)	3081-01-4	1,4-benzenediamine, N-(1,4-dimethylpentyl)-N′-phenyl-
PvB72	N	309-00-2	1,4:5,8-dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1.alpha.,4.alpha.,4a.beta.,5.alpha.,8.alpha.,8a.beta.)-
PvB73	N	3091-32-5	stannane, chlorotricyclohexyl-
PvB25	D(a)	3147-75-9	phenol, 2-(2H-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)-
PvB26	D(a)	32388-55-9	ethanone, 1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)-, [3R-(3alpha,3abeta,7beta,8aalpha)]-
PvB27	D(a)	3271-22-5	1,3,5-triazine, 2,4-dimethoxy-6-(1-pyrenyl)-
PvB28	D(a)	3278-89-5	benzene, 1,3,5-tribromo-2-(2-propenyloxy)-
PvB29	D(a)	335-57-9	heptane, hexadecafluoro-
PvB30	D(a)	3407-42-9	cyclohexanol, 3-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)-
PvB112	DSL-E	3468-63-1	2-naphthalenol, 1-[(2,4-dinitrophenyl)azo]-
PvB31	D(a)	355-42-0	hexane, tetradecafluoro-
PvB32	D(a)	355-43-1	hexane, 1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-6-iodo-
PvB33	D(a)	36437-37-3	phenol, 2-(2H-benzotriazol-2-yl)-4-(1,1-dimethylethyl)-6-(1-methylpropyl)-

Code number	Source	CAS	Substance
PvB92	O	36861-47-9	bicyclo(2.2.1)heptan-2-one, 1,7,7-trimethyl-3-[(4-methylphenyl)methylene]-
PvB34	D(a)	3739-67-1	benzene, 1,1′-(1-methylethylidene)bis[4-(2-propenyloxy)-
PvB84	O	375-72-4	1-butanesulfonyl fluoride, 1,1,2,2,3,3,4,4,4-nonafluoro-
PvB35	D(a)	3846-71-7	phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)-
PvB36	D(a)	38521-51-6	benzene, pentabromo(bromomethyl)-
PvB93	O	38521-51-6	benzene, pentabromo(bromomethyl)-
PvB75	N	3861-47-0	octanoic acid, 4-cyano-2,6-diiodophenyl ester
PvB37	D(a)	3864-99-1	phenol, 2-(5-chloro-2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)-
PvB76	N	40487-42-1	benzenamine, N-(1-ethylpropyl)-3,4-dimethyl-2,6-dinitro-
PvB87	O	4051-63-2	[1,1′-bianthracene]-9,9′,10,10′-tetrone, 4,4′-diamino-
PvB38	D(a)	40567-16-6	butanoyl chloride, 2-[2,4-bis(1,1-dimethylpropyl)phenoxy]-
PvB77	N	41083-11-8	1H-1,2,4-triazole, 1-(tricyclohexylstannyl)-
PvB39	D(a)	4130-42-1	phenol, 2,6-bis(1,1-dimethylethyl)-4-ethyl-
PvB40	D(a)	4162-45-2	ethanol, 2,2′-[(1-methylethylidene)bis[(2,6-dibromo-4,1-phenylene)oxy]]bis-
PvB95	O	41999-84-2	benzene, 1,4-dichloro-2,5-bis(dichloromethyl)-
PvB41	D(a)	42074-68-0	benzene, 1-chloro-2-(chlorodiphenylmethyl)-
PvB42	D(a)	423-50-7	1-hexanesulfonyl fluoride, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-
PvB113	DSL-E	42739-61-7	nickel, bis[2,3-bis(hydroxyimino)-N-(2-methoxyphenyl)butanamidato]-
PvB114	DSL-E	43035-18-3	benzenesulfonic acid, 4-[[3-[[2-hydroxy-3-[[(4-methoxyphenyl)amino]carbonyl]-1-naphthalenyl]azo]-4-methylbenzoyl]amino]-, calcium salt (2:1)
PvB43	D(a)	4378-61-4	dibenzo[def,mno]chrysene-6,12-dione, 4,10-dibromo-
PvB115	DSL-E	475-71-8	benzo[h]benz[5,6]acridino[2,1,9,8-klmna]acridine-8,16-dione
PvB45	D(a)	50772-29-7	butanoyl chloride, 4-[2,4-bis(1,1-dimethylpropyl)phenoxy]-
PvB116	DSL-E	509-34-2	spiro[isobenzofuran-1(3H),9′-[9H]xanthen]-3-one, 3′,6′-bis(diethylamino)-
PvB46	D(a)	512-04-9	spirost-5-en-3-ol, (3beta,25R)-
PvB47	D(a)	51630-58-1	benzeneacetic acid, 4-chloro-alpha-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester
PvB48	D(a)	5165-81-1	2-naphthalenecarboxamide, N-(4-chloro-2-methoxy-5-methylphenyl)-3-hydroxy-
PvB78	N	52315-07-8	cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester (cypermethrin)
PvB49	D(a)	52434-90-9	1,3,5-triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris(2,3-dibromopropyl)-
PvB117	DSL-E	5261-31-4	propanenitrile, 3-[[2-(acetyloxy)ethyl][4-[(2,6-dichloro-4-nitrophenyl)azo]phenyl]amino]-
PvB79	N	52645-53-1	cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, (3-phenoxyphenyl)methyl ester
PvB118	DSL-E	52697-38-8	acetamide, N-[2-[(2-bromo-4,6-dinitrophenyl)azo]-5-(diethylamino)phenyl]-
PvB50	D(a)	52740-90-6	2-anthracenecarboxamide, 1-amino-N-(3-bromo-9,10-dihydro-9,10-dioxo-2-anthracenyl)-9,10-dihydro-9,10-dioxo-
PvB51	D(a)	5285-60-9	benzenamine, 4,4′-methylenebis[N-(1-methylpropyl)-
PvB119	DSL-E	53184-75-1	phosphorous acid, (1-methylethylidene)di-4,1-phenylene tetrakis[(3-ethyl-3-oxetanyl)methyl] ester
PvB52	D(a)	54079-53-7	propanedinitrile, [[4-[[2-(4-cyclohexylphenoxy)ethyl]ethylamino]-2-methylphenyl]methylene]-

Code number	Source	CAS	Substance
PvB53	D(a)	54914-37-3	cyclohexanemethanamine, 1,3,3-trimethyl-N-(2-methylpropylidene)-5-[(2-methylpropylidene)amino]-
PvB54	D(a)	55525-54-7	urea, N,N′-bis[(5-isocyanato-1,3,3-trimethylcyclohexyl)methyl]-
PvB55	D(a)	56358-17-9	2-naphthalenamine, N-(2-ethylhexyl)-
PvB155	FR	58965-66-5	tetradecabromodiphenoxybenzene
PvB56	D(a)	59447-55-1	2-propenoic acid, (pentabromophenyl)methyl ester
PvB121	DSL-E	59487-23-9	2-naphthalenecarboxamide, 4-[[5-[[[4-(aminocarbonyl)phenyl]amino]carbonyl]-2-methoxyphenyl]azo]-N-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxy-
PvB122	DSL-E	59709-10-3	pyridinium, 1-[2-[[4-[(2-chloro-4-nitrophenyl)azo]phenyl]ethylamino]ethyl]-, acetate
PvB123	DSL-E	59709-38-5	β-alanine, N-[4-[(2-bromo-6-chloro-4-nitrophenyl)azo]phenyl]-N-(3-methoxy-3-oxopropyl)-, methyl ester
PvB80	N	61951-96-0	neodecanoic acid, cadmium salt
PvB158	UV	6197-30-4	octocrylene
PvB124	DSL-E	6250-23-3	phenol, 4-[[4-(phenylazo)phenyl]azo]-
PvB57	D(a)	63059-55-2	hexanoyl chloride, 2-[2,4-bis(1,1-dimethylpropyl)phenoxy]-
PvB58	D(a)	63216-89-7	1H-indene-1,3(2H)-dione, 2-benzo[f]quinolin-3-yl-
PvB85	O	632-79-1	1,3-isobenzofurandione, 4,5,6,7-tetrabromo-
PvB125	DSL-E	6407-78-9	3H-pyrazol-3-one, 4-[(2,4-dimethylphenyl)azo]-2,4-dihydro-5-methyl-2-phenyl-
PvB126	DSL-E	6410-41-9	2-naphthalenecarboxamide, N-(5-chloro-2,4-dimethoxyphenyl)-4-[[5-[(diethylamino)sulfonyl]-2-methoxyphenyl]azo]-3-hydroxy-
PvB127	DSL-E	64338-16-5	7-oxa-3,20-diazadispiro[5.1.11.2]heneicosan-21-one, 2,2,4,4-tetramethyl-
PvB149	F	65113-99-7	a,b,2,2,3-pentamethylcyclopent-3-ene-1-butanol
PvB128	DSL-E	65140-91-2	phosphonic acid, [[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-, monoethyl ester, calcium salt (2:1)
PvB129	DSL-E	6731-36-8	peroxide, (3,3,5-trimethylcyclohexylidene)bis[(1,1-dimethylethyl)
PvB81	N	67375-30-8	cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester (alpha-cypermethrin)
PvB130	DSL-E	6786-83-0	1-naphthalenemethanol, α,α-bis[4-(dimethylamino)phenyl]-4-(phenylamino)-
PvB143	HSE-R48	67-97-0	colecalciferol, Vitamin D3
PvB96	O	68085-85-8	cyclopropanecarboxylic acid, 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester
PvB131	DSL-E	68391-08-2	alcohols, C8–14, γ-ω-perfluoro
PvB132	DSL-E	68877-63-4	acetamide, N-[2-[(2-bromo-4,6-dinitrophenyl)azo]-5-[(2-cyanoethyl)-2-propenylamino]-4-methoxyphenyl]-
PvB133	DSL-E	70331-94-1	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, (1,2-dioxo-1,2-ethanediyl)bis(imino-2,1-ethanediyl) ester
PvB134	DSL-E	70660-55-8	1-naphthalenamine, 4-[(2-bromo-4,6-dinitrophenyl)azo]-N-(3-methoxypropyl)-
PvB88	O	7139-02-8	pyrimido[5,4-d]pyrimidine, 2,6-dichloro-4,8-di-1-piperidinyl-
PvB135	DSL-E	72869-85-3	chromate(1-), bis[3,5-bis(1,1-dimethylethyl)-2-hydroxybenzoato(2-)-O1,O2]-, hydrogen
PvB136	DSL-E	72968-82-2	methanesulfonamide, N-[2-[(2,6-dicyano-4-methylphenyl)azo]-5-(dipropylamino)phenyl]-
PvB59	D(a)	732-26-3	phenol, 2,4,6-tris(1,1-dimethylethyl)-
PvB137	DSL-E	74336-60-0	9,10-anthracenedione, 1-[(5,7-dichloro-1,9-dihydro-2-methyl-9-oxopyrazolo[5,1-b]quinazolin-3-yl)azo]-
PvB150	F	77-54-3	[3R-(3a,3ab,6a,7b,8aa)]-octahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl acetate
PvB138	DSL-E	78-63-7	peroxide, (1,1,4,4-tetramethyl-1,4-butanediyl)bis[(1,1-dimethylethyl)

Code number	Source	CAS	Substance
PvB82	O	81-98-1	7H-benz[de]anthracen-7-one, 3,9-dibromo-
PvB139	DSL-E	83006-67-1	benzenesulfonic acid, 2,2′-[(9,10-dihydro-5,8-dihydroxy-9,10-dioxo-1,4-anthracenediyl)diimino]bis[5-(1,1-dimethylethyl)-, disodium salt
PvB142	DSL-H	842-07-9	2-naphthalenol, 1-(phenylazo)-
PvB61	D(a)	850-92-0	1,3-cyclopentanedione, 2-[2-(3,4-dihydro-6-methoxy-1(2H)-naphthalenylidene)ethyl]-2-ethyl-
PvB62	D(a)	85-22-3	benzene, pentabromoethyl-
PvB140	DSL-E	85702-64-3	3H-indol-3-one, 5,7-dibromo-2-(5-bromo-7-chloro-1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-
PvB141	DSL-E	85-86-9	2-naphthalenol, 1-[[4-(phenylazo)phenyl]azo]-
PvB148	F	87-44-5	caryophyllene
PvB63	D(a)	87-83-2	benzene, pentabromomethyl-
PvB64	D(a)	90-93-7	methanone, bis[4-(diethylamino)phenyl]-
PvB65	D(a)	93-46-9	1,4-benzenediamine, N,N′-di-2-naphthalenyl-
PvB151	FR	96-69-5	4,4′-thio-bis(2-t-butyl-5-methylphenol)

Source: D(a), Danish EPA database R50/53; D(b), Danish EPA database R51/53+Mut3; N, N-Class; O, OSPAR list; DSL-E, Canadian PBiT list; DSL-H, Canadian PBiThuman list; HSE-R48, HSE R48 list; F, fragrance-sector report; FR, flame-retardants sector report; UV, UV-filters report. See Section 2.2 for more information.

Table A2.2 PB substances ordered by CAS number.

Code number	Source	CAS	Substance
PB23	D(b)	101-20-2	urea, N-(4-chlorophenyl)-N′-(3,4-dichlorophenyl)-
PB1	D(a)	10310-32-4	D-glucofuranoside, ethyl 3,5,6-tris-O-(phenylmethyl)-
PB27	O	116-29-0	benzene, 1,2,4-trichloro-5-[(4-chlorophenyl)sulfonyl]-
PB2	D(a)	119-94-8	benzenemethanamine, N-ethyl-N-(3-methylphenyl)-
PB36	F	127-51-5	3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one
PB3	D(a)	129-00-0	pyrene
PB35	F	1335-46-2	ionone, methyl-
PB4	D(a)	133-91-5	benzoic acid, 2-hydroxy-3,5-diiodo-
PB5	D(a)	15307-93-4	benzenamine, 2,6-dichloro-N-phenyl-
PB30	DSL-E	1937-37-7	2,7-naphthalenedisulfonic acid, 4-amino-3-[[4′-[(2,4-diaminophenyl)azo][1,1′-biphenyl]-4-yl]azo]-5-hydroxy-6-(phenylazo)-, disodium salt
PB31	DSL-E	2778-42-9	benzene, 1,3-bis(1-isocyanato-1-methylethyl)-
PB6	D(a)	3380-34-5	phenol, 5-chloro-2-(2,4-dichlorophenoxy)-
PB25	N	41198-08-7	profenofos
PB7	D(a)	41604-19-7	1,1′-biphenyl, 4-bromo-2-fluoro-
PB8	D(a)	4273-92-1	2-naphthalenecarboxamide, N-(4-chloro-2,5-dimethoxyphenyl)-3-hydroxy-
PB9	D(a)	43076-61-5	1-butanone, 4-chloro-1-[4-(1,1-dimethylethyl)phenyl]-
PB10	D(a)	464-41-5	bicyclo[2.2.1]heptane, 2-chloro-1,7,7-trimethyl-, endo-
PB11	D(a)	467-63-0	benzenemethanol, 4-(dimethylamino)-alpha,alpha-bis[4-(dimethylamino)phenyl]-
PB26	O	50-63-5	1,4-pentanediamine, N(4)-(7-chloro-4-quinolinyl)-N(1),N(1)-diethyl-, phosphate (1:2)
PB12	D(a)	50-65-7	benzamide, 5-chloro-N-(2-chloro-4-nitrophenyl)-2-hydroxy-
PB13	D(a)	51-03-6	1,3-benzodioxole, 5-[[2-(2-butoxyethoxy)ethoxy]methyl]-6-propyl-
PB28	O	52179-28-9	propanoic acid, 2-[4-(2,2-dichlorocyclopropyl)phenoxy]-2-methyl-, ethyl ester
PB32	DSL-E	56-95-1	2,4,11,13-tetraazatetradecanediimidamide, N,N″-bis(4-chlorophenyl)-3,12-diimino-, diacetate
PB14	D(a)	57018-04-9	phosphorothioic acid, O-(2,6-dichloro-4-methylphenyl) O,O-dimethyl ester
PB15	D(a)	626-39-1	benzene, 1,3,5-tribromo-
PB16	D(a)	634-66-2	benzene, 1,2,3,4-tetrachloro-
PB17	D(a)	63734-62-3	benzoic acid, 3-[2-chloro-4-(trifluoromethyl)phenoxy]-
PB18	D(a)	66063-05-6	urea, N-[(4-chlorophenyl)methyl]-N-cyclopentyl-N′-phenyl-
PB29	O	68015-60-1	benzenesulfonic acid, 2-amino-, (1-methylethylidene)di-4,1-phenylene ester

Code number	Source	CAS	Substance
PB33	DSL-E	72828-93-4	1-propanaminium, 3-[[9,10-dihydro-4-[(4-methylphenyl)amino]-9,10-dioxo-1-anthracenyl]amino]-N,N,N-trimethyl-, methyl sulfate
PB19	D(a)	7785-70-8	bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-, (1R)-
PB34	DSL-E	81-68-5	benzenesulfonamide, N-(4-amino-9,10-dihydro-3-methoxy-9,10-dioxo-1-anthracenyl)-4-methyl-
PB20	D(a)	82-05-3	7H-benz[de]anthracen-7-one
PB22	D(a)	92-72-8	2-naphthalenecarboxamide, N-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxy-

Source: D(a), Danish EPA database R50/53; D(b), Danish EPA database R51/53+Mut3; N, N-Class; O, OSPAR list; DSL-E, Canadian PBiT list; F, fragrance-sector report. See Section 2.2 for more information.

Project code no.	PvB1				
Substance name	Benzene, 1,1'-(1,2-diethyl-1,2-dimethyl-1,2-ethanediyl)bis-				
Synonyms					
CAS No	10192-93-5	EINECS No		233-474-4	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.46	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00045				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.008			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has use as synergist for fire retardants				
Potential for exposure over wide scale?	Yes, based on confidential use information and on *Kirk-Othmer* information				
Overall comments	High priority for further investigation				

Project code no.	PvB2				
Substance name	Benzenamine, 4-dodecyl-				
Synonyms					
CAS No	104-42-7	EINECS No		203-201-3	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)	Readily biodegradable			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured result accepted by regulatory authority				
Log K_{ow}	7.03	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00032				ECOSAR
Ecotoxicity comment	T from Danish EPA predictions				
Water solubility (mg/l)	0.02			WS source	EPI SUITE
P classification	Not P (based on measured value)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Not PBT				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Low priority for further investigation				

Project code no.	PvB3				
Substance name	Cedrene				
Synonyms					
CAS No	11028-42-5		EINECS No	234-257-7	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.74	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.011				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.15			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* and web have use in fragrances				
Potential for exposure over wide scale?	Yes, based on confidential use information, and on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB4				
Substance name	Decane, 1-bromo				
Synonyms					
CAS No	112-29-8		EINECS No	203-995-3	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.6	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.016				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.56			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB7				
Substance name	Benzenamine, 4,4'-(phenylmethylene)bis[N,N-dimethyl-				
Synonyms					
CAS No	129-73-7	EINECS No		204-961-9	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.31	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.018				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.10			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB8				
Substance name	1-Phenanthrenemethanol, tetradecahydro-1,4a-dimethyl-7-(1-methylethyl)-				
Synonyms					
CAS No	13393-93-6		EINECS No	236-476-3	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.4	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.004				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.15			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, as no suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB9				
Substance name	Benzenamine, 4,4'-methylenebis[N,N-diethyl-				
Synonyms					
CAS No	135-91-1	EINECS No	205-224-4		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.34	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.005				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.04			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB10				
Substance name	Benzenamine, 4,4'-methylenebis[2,6-diethyl-				
Synonyms					
CAS No	13680-35-8	EINECS No		237-185-4	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.34	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00103				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.04			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB11				
Substance name	1,4-Benzenediamine, N,N'-bis(1-ethyl-3-methylpentyl)-				
Synonyms					
CAS No	139-60-6	EINECS No		205-368-8	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.29	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.000794				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.005			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	*Kirk-Othmer* has commercial antioxidant and ozonant				
Potential for exposure over wide scale?	Yes, based on confidential use information and on *Kirk-Othmer* information				
Overall comments	High priority for further investigation				

Project code no.	PvB12				
Substance name	9H-Carbazole, 9-butyl-				
Synonyms					
CAS No	1484-08-8	EINECS No		216-051-9	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.31	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.028				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.07			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential information				
Overall comments	High priority for further investigation				

Project code no.	PvB13				
Substance name	1,4-Benzenediamine, N-(1-methylheptyl)-N'-phenyl-				
Synonyms					
CAS No	15233-47-3	EINECS No	239-281-1		
Existing regulatory and related activity (e.g. priority lists)	US HPV				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	5.74	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.016				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.16			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	*Kirk-Othmer* has use as antioxidant				
Potential for exposure over wide scale?	Yes, based on confidential use information and on *Kirk-Othmer* information				
Overall comments	High priority for further investigation				

Project code no.	PvB15				
Substance name	Phenol, 2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-				
Synonyms					
CAS No	17540-75-9	EINECS No	241-533-0		
Existing regulatory and related activity (e.g. priority lists)	OSPAR, Canadian DSL, US HPV				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	6.43	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.003				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.25			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB17				
Substance name	Benzene, 1,1'-(1,1,2,2-tetramethyl-1,2-ethanediyl)bis-				
Synonyms					
CAS No	1889-67-4	EINECS No	217-568-2		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.48	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.003				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.07			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has use as fire-retardant synergist				
Potential for exposure over wide scale?	Yes, based on confidential use information and on *Kirk-Othmer* information				
Overall comments	High priority for further investigation				

Project code no.	PvB18				
Substance name	1-Phenanthrenecarboxylic acid, tetradecahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1alpha,4abeta,4balpha,7beta,8abeta,10aalpha)]-				
Synonyms					
CAS No	19941-28-7		EINECS No	243-435-3	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.92	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00157				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.01			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes from confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB19				
Substance name	1H-Imidazole, 1-[(2-chlorophenyl)diphenylmethyl]-				
Synonyms	Clotrimazole				
CAS No	23593-75-1		EINECS No	245-764-8	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.26	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.023			Ecotox source	ECOSAR
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.03			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, on web				
Summary of use	OSPAR indicates use as drug				
Potential for exposure over wide scale?	Yes, from use information				
Overall comments	High priority for further investigation				

Project code no.	PvB20				
Substance name	Benzene, 1,1',1''-methylidynetris[4-isocyanato-				
Synonyms					
CAS No	2422-91-5	EINECS No	219-351-8		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.17	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	No predicted value				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.004			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB21				
Substance name	Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)-				
Synonyms					
CAS No	25973-55-1	EINECS No	247-384-8		
Existing regulatory and related activity (e.g. priority lists)	OSPAR, US HPV				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	7.25	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF	2400	BCF data type	Measured	BCF source	CHRIP
Lowest acute ecotox L(E)C50 (mg/l)	No effects at solubility			Ecotox source	HPVIS
Lowest chronic ecotox NOEC (mg/l)	0.000743				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions; predicted classification used				
Water solubility (mg/l)	0.01			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (based on measured result accepted by regulatory authority)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has use in coatings				
Potential for exposure over wide scale?	Yes, based on confidential use information and on *Kirk-Othmer* information				
Overall comments	High priority for further investigation				

Project code no.	PvB22				
Substance name	Benzenamine, 4-(2,6-diphenyl-4-pyridinyl)-N,N-dimethyl-				
Synonyms					
CAS No	29312-59-2		EINECS No	249-551-0	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.27	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.006				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.03			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB23				
Substance name	[1,1'-Biphenyl]-4,4'-diamine, N,N'-bis(2,4-dinitrophenyl)-3,3'-dimethoxy-				
Synonyms					
CAS No	29398-96-7		EINECS No	249-605-3	
Existing regulatory and related activity (e.g. priority lists)	OSPAR, Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.94	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.000966				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.0003			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB24				
Substance name	1,4-Benzenediamine, N-(1,4-dimethylpentyl)-N'-phenyl-				
Synonyms					
CAS No	3081-01-4		EINECS No	221-374-3	
Existing regulatory and related activity (e.g. priority lists)	OSPAR, US HPV				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.17	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.2			Ecotox source	CHIRP
Lowest chronic ecotox NOEC (mg/l)	0.047				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.67			WS source	US HPV
P classification	P (provisional)				
B classification	vB (provisional				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB25				
Substance name	Phenol, 2-(2H-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)-				
Synonyms					
CAS No	3147-75-9	EINECS No		221-573-5	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.21	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	16			Ecotox source	US HPV
Lowest chronic ecotox NOEC (mg/l)	0.004				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.17			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has use as UV stabiliser				
Potential for exposure over wide scale?	Yes, based on confidential use information and on *Kirk-Othmer* information				
Overall comments	High priority for further investigation				

Project code no.	PvB26				
Substance name	Ethanone, 1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)-, [3R-(3alpha,3abeta,7beta,8aalpha)]-				
Synonyms	Methyl cedryl ketone				
CAS No	32388-55-9	EINECS No		251-020-3	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.02	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.044				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	1.28			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	Web information indicated use in fragrances				
Potential for exposure over wide scale?	Yes, based on confidential use information and on web information				
Overall comments	High priority for further investigation				

Project code no.	PvB27				
Substance name	1,3,5-Triazine, 2,4-dimethoxy-6-(1-pyrenyl)-				
Synonyms					
CAS No	3271-22-5	EINECS No		221-896-1	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.46	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.004				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.002			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has use as fabric brightener				
Potential for exposure over wide scale?	Yes, based on confidential use information and *Kirk-Othmer* information				
Overall comments	High priority for further investigation				

Project code no.	PvB28				
Substance name	Benzene, 1,3,5-tribromo-2-(2-propenyloxy)-				
Synonyms					
CAS No	3278-89-5		EINECS No	221-913-2	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.59	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.03				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.08			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	Web information indicates use as a flame retardant				
Potential for exposure over wide scale?	Yes, based on confidential use information and on web information				
Overall comments	High priority for further investigation				

Project code no.	PvB29				
Substance name	Heptane, hexadecafluoro-				
Synonyms					
CAS No	335-57-9	EINECS No		206-392-1	
Existing regulatory and related activity (e.g. priority lists)	OSPAR, US HPV				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.99	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF	8740	BCF data type	Measured	BCF source	CHRIP
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00169				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.0007			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (based on measured result accepted by regulatory authority)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No definite use information, so assume yes				
Overall comments	High priority for further investigation				

Project code no.	PvB30				
Substance name	Cyclohexanol, 3-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)-				
Synonyms					
CAS No	3407-42-9	EINECS No		222-294-1	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.5	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.02				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	1.82			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, on web				
Summary of use	Raw material in fragrances (web)				
Potential for exposure over wide scale?	Yes, based on confidential use information and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB31				
Substance name	Hexane, tetradecafluoro-				
Synonyms					
CAS No	355-42-0	EINECS No		206-585-0	
Existing regulatory and related activity (e.g. priority lists)	OSPAR, US HPV				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.02	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	No effects at solubility			Ecotox source	US HPV
Lowest chronic ecotox NOEC (mg/l)	0.01				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.009			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, on web				
Summary of use	Heat-transfer agent in electronics industry (*Kirk-Othmer*)				
Potential for exposure over wide scale?	Yes, based on confidential use information and *Kirk-Othmer* information				
Overall comments	High priority for further investigation; Log K_{ow} may be unreliable as an indicator of bioaccumulation potential for this type of substance				

Project code no.	PvB32				
Substance name	Hexane, 1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-6-iodo-				
Synonyms					
CAS No	355-43-1	EINECS No		206-586-6	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.84	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.003				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.0004			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation; Log K_{ow} may be unreliable as an indicator of bioaccumulation potential for this type of substance				

Project code no.	PvB33				
Substance name	Phenol, 2-(2H-benzotriazol-2-yl)-4-(1,1-dimethylethyl)-6-(1-methylpropyl)-				
Synonyms					
CAS No	36437-37-3		EINECS No	253-037-1	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	6.31	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF	13,000	BCF data type	Measured	BCF source	CHRIP
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.003				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.14			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (based on measured result accepted by regulatory authority)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	UV absorber, light stabiliser (web)				
Potential for exposure over wide scale?	Yes, based on confidential use information and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB34				
Substance name	Benzene, 1,1'-(1-methylethylidene)bis[4-(2-propenyloxy)-				
Synonyms					
CAS No	3739-67-1	EINECS No	223-123-3		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.46	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.007				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.03			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4 and on web				
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB35				
Substance name	Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)-				
Synonyms					
CAS No	3846-71-7	EINECS No	223-346-6		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	6.27	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF	10,000	BCF data type	Measured	BCF source	CHRIP
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.003				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.15			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (based on measured result accepted by regulatory authority)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB36				
Substance name	Benzene, pentabromo(bromomethyl)-				
Synonyms					
CAS No	38521-51-6	EINECS No	253-985-6		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.33	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	No predicted value				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.0001			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB37				
Substance name	Phenol, 2-(5-chloro-2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)-				
Synonyms					
CAS No	3864-99-1	EINECS No	223-383-8		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	6.91	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF	7600	BCF data type	Measured	BCF source	CHRIP
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.0013				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.03			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional) (but note that EURAS BCF gold-standard database has much lower values of 12.3 and 15.9)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* and web have use as UV stabiliser				
Potential for exposure over wide scale?	Yes, based on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB38				
Substance name	Butanoyl chloride, 2-[2,4-bis(1,1-dimethylpropyl)phenoxy]-				
Synonyms					
CAS No	40567-16-6	EINECS No	254-978-0		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.48	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	No predicted value				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.02			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information and no current suppliers identified				
Overall comments	Medium priority for further investigation				

Project code no.	PvB39				
Substance name	Phenol, 2,6-bis(1,1-dimethylethyl)-4-ethyl-				
Synonyms					
CAS No	4130-42-1		EINECS No	223-945-2	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	5.52	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF	5060 4,900; 5,010	BCF data type	Measured Measured	BCF source	CHRIP EURAS
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.007				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	2.1			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (based on measured result accepted by regulatory authority and on gold-standard BCF database)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	Anti-oxidant in *Kirk-Othmer* and on web				
Potential for exposure over wide scale?	Yes, based on confidential use information, and on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB40				
Substance name	Ethanol, 2,2'-[(1-methylethylidene)bis[(2,6-dibromo-4,1-phenylene)oxy]]bis-				
Synonyms	Tetrabromobisphenol-A bis(2-hydroxyethylether)				
CAS No	4162-45-2	EINECS No		224-005-4	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.78	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF	250	BCF data type	Measured	BCF source	CHRIP
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.004				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.0002			WS source	EPI SUITE
P classification	P (provisional)				
B classification	Not B (based on measured result accepted by regulatory authority, and other lower values from EURAS BCF gold-standard database)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Not PBT as does not meet B criterion				
Possible UK suppliers (with source)	Yes, in IUCLID and on web				
Summary of use	Reactive flame retardant in *Kirk-Othmer*				
Potential for exposure over wide scale?	No, based on confidential use information and on *Kirk-Othmer* information				
Overall comments	Low priority, as not PBT and low exposure use; previously flagged as potential PBT in EA (2003)				

Project code no.	PvB41				
Substance name	Benzene, 1-chloro-2-(chlorodiphenylmethyl)-				
Synonyms					
CAS No	42074-68-0		EINECS No	255-647-3	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.23	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	No predicted value				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.05			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	Use in chemical synthesis, on web				
Potential for exposure over wide scale?	No, based on confidential use information and web information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB42				
Substance name	1-Hexanesulfonyl fluoride, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-				
Synonyms					
CAS No	423-50-7	EINECS No	207-026-3		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.68	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	No predicted value				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.0008			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, on web				
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation; Log K_{ow} may be unreliable as an indicator of bioaccumulation potential for this type of substance				

Project code no.	PvB43				
Substance name	Dibenzo[def,mno]chrysene-6,12-dione, 4,10-dibromo-				
Synonyms					
CAS No	4378-61-4	EINECS No	224-481-3		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.13	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	ECOSAR
Lowest chronic ecotox NOEC (mg/l)	0.00153				
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.00008			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	Dye and/or pigment based, based on web information				
Potential for exposure over wide scale?	Yes, based on confidential use information and on web information				
Overall comments	High priority for further investigation				

Project code no.	PvB45				
Substance name	Butanoyl chloride, 4-[2,4-bis(1,1-dimethylpropyl)phenoxy]-				
Synonyms					
CAS No	50772-29-7	EINECS No	256-755-3		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.55	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	No predicted value				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	1.7			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, as IUCLID entry indicates ceased production and no current suppliers found				
Overall comments	Medium priority for further investigation				

Project code no.	PvB46				
Substance name	Spirost-5-en-3-ol, (3beta,25R)-				
Synonyms	Diosgenin				
CAS No	512-04-9	EINECS No	208-134-3		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.34	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.007				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.03			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, on web				
Summary of use	OSPAR has use as hormone				
Potential for exposure over wide scale?	Yes, based on OSPAR and web information				
Overall comments	High priority for further investigation; this is a plant-derived steroidal compound				

Project code no.	PvB47				
Substance name	Benzeneacetic acid, 4-chloro-alpha-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester				
Synonyms	Fenvalerate				
CAS No	51630-58-1	EINECS No			
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.76	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.003				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.006			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	OSPAR and *Kirk-Othmer* have use as pesticide				
Potential for exposure over wide scale?	Yes, based on OSPAR, *Kirk-Othmer* and confidential information				
Overall comments	High priority for further investigation				

Project code no.	PvB48				
Substance name	2-Naphthalenecarboxamide, N-(4-chloro-2-methoxy-5-methylphenyl)-3-hydroxy-				
Synonyms					
CAS No	5165-81-1		EINECS No	225-946-3	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.18	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.015				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.99			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	Web supplier in China states use in colourants				
Potential for exposure over wide scale?	Not clear, assume yes				
Overall comments	High priority for further investigation				

Project code no.	PvB49				
Substance name	1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris(2,3-dibromopropyl)-				
Synonyms					
CAS No	52434-90-9		EINECS No	257-913-4	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.37	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	No predicted value				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.00001			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has use as additive flame retardant				
Potential for exposure over wide scale?	Yes, based on confidential use information and on *Kirk-Othmer* information				
Overall comments	High priority for further investigation				

Project code no.	PvB50				
Substance name	2-Anthracenecarboxamide, 1-amino-N-(3-bromo-9,10-dihydro-9,10-dioxo-2-anthracenyl)-9,10-dihydro-9,10-dioxo-				
Synonyms					
CAS No	52740-90-6	EINECS No		258-148-9	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.83	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.0009				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.00004			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB51				
Substance name	Benzenamine, 4,4'-methylenebis[N-(1-methylpropyl)-				
Synonyms					
CAS No	5285-60-9	EINECS No	226-122-6		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.08	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.008				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.07			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB52				
Substance name	Propanedinitrile, [[4-[[2-(4-cyclohexylphenoxy)ethyl]ethylamino]-2-methylphenyl]methylene]-				
Synonyms					
CAS No	54079-53-7		EINECS No	258-964-5	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.88	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.004			Ecotox source	ECOSAR
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.0002			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, as no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB53				
Substance name	Cyclohexanemethanamine, 1,3,3-trimethyl-N-(2-methylpropylidene)-5-[(2-methylpropylidene)amino]-				
Synonyms					
CAS No	54914-37-3		EINECS No	259-393-4	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.16	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.004			Ecotox source	ECOSAR
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.01			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information and no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB54				
Substance name	Urea, N,N'-bis[(5-isocyanato-1,3,3-trimethylcyclohexyl)methyl]-				
Synonyms					
CAS No	55525-54-7		EINECS No	259-695-6	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.31	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00096				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.001			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, as no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB55				
Substance name	2-Naphthalenamine, N-(2-ethylhexyl)-				
Synonyms					
CAS No	56358-17-9	EINECS No	260-126-9		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.16	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.006				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.12			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information and no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB56				
Substance name	2-Propenoic acid, (pentabromophenyl)methyl ester				
Synonyms					
CAS No	59447-55-1		EINECS No	261-767-7	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.89	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00135				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.0004			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has reactive flame retardant				
Potential for exposure over wide scale?	No, based on confidential use information and *Kirk-Othmer* information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB57				
Substance name	Hexanoyl chloride, 2-[2,4-bis(1,1-dimethylpropyl)phenoxy]-				
Synonyms					
CAS No	63059-55-2		EINECS No	263-825-7	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.46	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.009			Ecotox source	ECOSAR
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.002			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, as no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB58				
Substance name	1H-Indene-1,3(2H)-dione, 2-benzo[f]quinolin-3-yl-				
Synonyms					
CAS No	63216-89-7		EINECS No	264-007-2	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.39	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.035				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.02			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, as no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB59				
Substance name	Phenol, 2,4,6-tris(1,1-dimethylethyl)-				
Synonyms					
CAS No	732-26-3	EINECS No	211-989-5		
Existing regulatory and related activity (e.g. priority lists)	OSPAR, Canadian DSL				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	6.39 6.06	K_{ow} data type	Predicted Measured	Log K_{ow} source	EPI SUITE US HPV
BCF	23,400	BCF data type	Measured	BCF source	EURAS
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.003				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.51			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (similar values in CHRIP)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4 and on web				
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation; further information is available in an OSPAR Commission background document from 2006, and a Canadian Government Screening Assessment from 2008				

Project code no.	PvB61				
Substance name	1,3-Cyclopentanedione, 2-[2-(3,4-dihydro-6-methoxy-1(2H)-naphthalenylidene)ethyl]-2-ethyl-				
Synonyms					
CAS No	850-92-0		EINECS No	212-705-2	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.33	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.038				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.29			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, as no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB62				
Substance name	Benzene, pentabromoethyl-				
Synonyms					
CAS No	85-22-3	EINECS No		201-593-0	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.48	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.000816				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.0003			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, on web				
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB63				
Substance name	Benzene, pentabromomethyl-				
Synonyms					
CAS No	87-83-2	EINECS No		201-774-4	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	6.99	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF	39	BCF data type	Measured	BCF source	EURAS, CHRIP
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	ECOSAR
Lowest chronic ecotox NOEC (mg/l)	0.002				
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.0009			WS source	EPI SUITE
P classification	P (provisional)				
B classification	Not B (based on measured result accepted by regulatory authority and included in gold-standard database)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Not PBT				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has use as additive flame retardant				
Potential for exposure over wide scale?	Yes, based on confidential use information and on *Kirk-Othmer* information				
Overall comments	Low priority for further investigation; previously flagged as potential PBT in EA (2003)				

Project code no.	PvB64				
Substance name	Methanone, bis[4-(diethylamino)phenyl]-				
Synonyms					
CAS No	90-93-7		EINECS No	202-025-4	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.47	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.03				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.19			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB65				
Substance name	1,4-Benzenediamine, N,N'-di-2-naphthalenyl-				
Synonyms					
CAS No	93-46-9	EINECS No	202-249-2		
Existing regulatory and related activity (e.g. priority lists)	OSPAR, Canadian DSL				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	6.39	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.005				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.001			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB66				
Substance name	8,16-Pyranthrenedione				
Synonyms	Vat Gold Orange G, Vat Orange 9, CI Pigment 40/41				
CAS No	128-70-1	EINECS No	204-906-9		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	8.05	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00212				ECOSAR
Ecotoxicity comments					
Water solubility (mg/l)	0.00003			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB (T from Danish EPA mutagenicity prediction)				
Possible UK suppliers (with source)					
Summary of use	Web information indicates use as dye				
Potential for exposure over wide scale?	Yes, based on confidential use information and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB67				
Substance name	2-Naphthalenecarboxamide, 3-hydroxy-N-(3-nitrophenyl)-				
Synonyms					
CAS No	135-65-9		EINECS No	205-209-2	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.01	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.017				ECOSAR
Ecotoxicity comments	(ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.9			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB (T from Danish EPA mutagenicity prediction)				
Possible UK suppliers (with source)					
Summary of use	Web information indicates use as an intermediate				
Potential for exposure over wide scale?	No, based on confidential use information and web information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB68				
Substance name	Stannane, tricyclohexylhydroxy-				
Synonyms	Cyhexatin				
CAS No	13121-70-5		EINECS No	236-049-1	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.63	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.003				ECOSAR
Ecotoxicity comments	T from N-Class entry				
Water solubility (mg/l)	0.008			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	OSPAR and web have use as pesticide				
Potential for exposure over wide scale?	Yes, based on OSPAR and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB69				
Substance name	Distannoxane, hexakis(2-methyl-2-phenylpropyl)-				
Synonyms	Fenbutatin oxide				
CAS No	13356-08-6	EINECS No	236-407-7		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	14.65	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	1×10^{-9}				ECOSAR
Ecotoxicity comments	T from N-Class entry				
Water solubility (mg/l)	$<1 \times 10^{-8}$			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	OSPAR and web have use as pesticide				
Potential for exposure over wide scale?	Yes, based on OSPAR and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB70				
Substance name	Octanoic acid, lead salt				
Synonyms					
CAS No	15696-43-2	EINECS No		239-790-9	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.82	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.022				ECOSAR
Ecotoxicity comments	T from N-Class entry (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.008			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, as no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB71				
Substance name	Octadecanoic acid, cadmium salt				
Synonyms					
CAS No	2223-93-0	EINECS No		218-743-6	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.38	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	No predicted value				ECOSAR
Ecotoxicity comments	T from N-Class entry				
Water solubility (mg/l)	0.002			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has use as plastics additive (stabiliser)				
Potential for exposure over wide scale?	Yes, based on confidential use information and *Kirk-Othmer* information				
Overall comments	High priority for further investigation				

Project code no.	PvB72				
Substance name	1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1.alpha.,4.alpha.,4a.beta.,5.alpha.,8.alpha.,8a.beta.)-				
Synonyms	Aldrin				
CAS No	309-00-2	EINECS No	206-215-8		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.75	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF	20,000	BCF data type	Measured	BCF source	EURAS, CHRIP
Lowest acute ecotox L(E)C50 (mg/l)	0.006			Ecotox source	ECOSAR
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	T from N-Class entry				
Water solubility (mg/l)	0.18 (measured)			WS source	CHRIP
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	OSPAR and web have use as pesticide				
Potential for exposure over wide scale?	Yes, based on OSPAR and web information				
Overall comments	High priority for further information				

Project code no.	PvB73				
Substance name	Stannane, chlorotricyclohexyl-				
Synonyms					
CAS No	3091-32-5		EINECS No	221-437-5	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.09	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00144				ECOSAR
Ecotoxicity comments	T from N-Class entry				
Water solubility (mg/l)	0.003			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB75				
Substance name	Octanoic acid, 4-cyano-2,6-diiodophenyl ester				
Synonyms	Ioxynil octanoate				
CAS No	3861-47-0	EINECS No	223-375-4		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.42	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.006				ECOSAR
Ecotoxicity comments	T from N-Class entry				
Water solubility (mg/l)	0.001			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4 and on web				
Summary of use	Web information has use as pesticide				
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB76				
Substance name	Benzenamine, N-(1-ethylpropyl)-3,4-dimethyl-2,6-dinitro-				
Synonyms	Pendimethalin				
CAS No	40487-42-1	EINECS No	254-938-2		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.18	K_{ow} data type	Measured	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.003				ECOSAR
Ecotoxicity comments	T from N-Class entry				
Water solubility (mg/l)	0.275 (measured)			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* and web have use as herbicide				
Potential for exposure over wide scale?	Yes, based on confidential information, and on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB77				
Substance name	1H-1,2,4-Triazole, 1-(tricyclohexylstannyl)-				
Synonyms	Azocyclotin				
CAS No	41083-11-8		EINECS No	255-209-1	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.39	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.047				ECOSAR
Ecotoxicity comments	T from N-Class entry (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.12 (measured)			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	Web information has use as an acaricide				
Potential for exposure over wide scale?	Yes, based on confidential use information and on web information				
Overall comments	High priority for further investigation				

Project code no.	PvB78				
Substance name	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester				
Synonyms	Cypermethrin				
CAS No	52315-07-8		EINECS No	257-842-9	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.38	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.0015			Ecotox source	ECOSAR
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	T from N-Class entry				
Water solubility (mg/l)	0.004 (measured)			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	Web has use as a pesticide				
Potential for exposure over wide scale?	Yes, based on web information				
Overall comments	High priority for further investigation				

Project code no.	PvB79				
Substance name	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, (3-phenoxyphenyl)methyl ester				
Synonyms	Permethrin				
CAS No	52645-53-1	EINECS No	258-067-9		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.43	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00073				ECOSAR
Ecotoxicity comments	T from N-Class entry				
Water solubility (mg/l)	0.006 (measured)			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4 and on web				
Summary of use	*Kirk-Othmer* and web information have use as an insecticide				
Potential for exposure over wide scale?	Yes, based on confidential use information, and on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB80				
Substance name	Neodecanoic acid, cadmium salt				
Synonyms					
CAS No	61951-96-0	EINECS No	263-352-6		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.54	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.005				ECOSAR
Ecotoxicity comments	T from N-Class entry				
Water solubility (mg/l)	0.004			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB81				
Substance name	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester				
Synonyms	Alpha-cypermethrin				
CAS No	67375-30-8	EINECS No	257-842-9		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.38	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.0015			Ecotox source	ECOSAR
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	T from N-Class entry				
Water solubility (mg/l)	0.004 (measured)			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, on web				
Summary of use	Web has use as pesticide				
Potential for exposure over wide scale?	Yes, based on web information				
Overall comments	High priority for further investigation				

Project code no.	PvB82				
Substance name	7H-Benz[de]anthracen-7-one, 3,9-dibromo-				
Synonyms					
CAS No	81-98-1	EINECS No	201-391-2		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.51	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.004				ECOSAR
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity				
Water solubility (mg/l)	0.0008			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* and web have use as intermediate for dyes				
Potential for exposure over wide scale?	No, based on *Kirk-Othmer* and web information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB83				
Substance name	Perylo[3,4-cd:9,10-c'd']dipyran-1,3,8,10-tetrone				
Synonyms					
CAS No	128-83-6	EINECS No		204-911-6	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.81	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00688				ECOSAR
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity				
Water solubility (mg/l)	0.0003			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, as no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB84				
Substance name	1-Butanesulfonyl fluoride, 1,1,2,2,3,3,4,4,4-nonafluoro-				
Synonyms					
CAS No	375-72-4	EINECS No		206-792-6	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.75	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	No predicted value				ECOSAR
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity				
Water solubility (mg/l)	0.15			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation. Log K_{ow} may be unreliable as an indicator of bioaccumulation potential for this type of substance.				

Project code no.	PvB85				
Substance name	1,3-Isobenzofurandione, 4,5,6,7-tetrabromo-				
Synonyms	Tetrabromophthalic anhydride				
CAS No	632-79-1		EINECS No	211-185-4	
Existing regulatory and related activity (e.g. priority lists)	OSPAR, US HPV				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Rapidly hydrolysed to tetrabromophthalic acid (NIEHS)				
Log K_{ow}	5.63	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.031				ECOSAR
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.02			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	*Kirk-Othmer* has use as a flame retardant				
Potential for exposure over wide scale?	Yes, based on confidential use information and *Kirk-Othmer* information				
Overall comments	Not identified as a PBT in EA (2003); low priority for further investigation based on rapid hydrolysis (the degradation product is not expected to have PBT properties)				

Project code no.	PvB86				
Substance name	Benzenamine, N-butyl-N-ethyl-2,6-dinitro-4-(trifluoromethyl)-				
Synonyms	Benfluralin				
CAS No	1861-40-1	EINECS No	217-465-2		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.31	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.003				ECOSAR
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity				
Water solubility (mg/l)	0.1 (measured)			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, on web				
Summary of use	*Kirk-Othmer* and web have use as herbicide				
Potential for exposure over wide scale?	Yes, based on confidential use information, and on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB87				
Substance name	[1,1'-Bianthracene]-9,9',10,10'-tetrone, 4,4'-diamino-				
Synonyms					
CAS No	4051-63-2		EINECS No	223-754-4	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.83	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00073				ECOSAR
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity				
Water solubility (mg/l)	0.0002			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB88				
Substance name	Pyrimido[5,4-d]pyrimidine, 2,6-dichloro-4,8-di-1-piperidinyl-				
Synonyms					
CAS No	7139-02-8		EINECS No	230-437-4	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.45	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.035				ECOSAR
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.1			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB89				
Substance name	9,10-Anthracenedione, 4,8-diamino-2-(4-ethoxyphenyl)-1,5-dihydroxy-				
Synonyms					
CAS No	15114-15-5		EINECS No	239-167-1	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.94	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.002				ECOSAR
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity				
Water solubility (mg/l)	0.002			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID but no current suppliers located				
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB90				
Substance name	Methanone, (2-butyl-3-benzofuranyl)[4-[2-(diethylamino)ethoxy]-3,5-diiodophenyl]-, hydrochloride				
Synonyms					
CAS No	19774-82-4		EINECS No	243-293-2	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	8.81	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.00138			Ecotox source	ECOSAR
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity				
Water solubility (mg/l)	0.0002			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB91				
Substance name	Benzene, 1,1'-(1-methylethylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)-				
Synonyms	Tetrabromobisphenol-A bis(2,3-dibromopropyl) ether				
CAS No	21850-44-2	EINECS No	244-617-5		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	11.52	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF	130	BCF data type	Measured	BCF source	CHRIP
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	7×10^{-6}				ECOSAR
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity				
Water solubility (mg/l)	$<1 \times 10^{-5}$			WS source	EPI SUITE
P classification	P (provisional)				
B classification	Not B (based on measured result accepted by regulatory authority)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Not PBT				
Possible UK suppliers (with source)	Yes, in IUCLID 4 (site now closed)				
Summary of use	*Kirk-Othmer* has additive flame retardant				
Potential for exposure over wide scale?	Yes, based on confidential use information and *Kirk-Othmer* information				
Overall comments	Low priority for further investigation; previously flagged as potential PBT in EA (2003)				

Project code no.	PvB92				
Substance name	Bicyclo(2.2.1)heptan-2-one, 1,7,7-trimethyl-3-[(4-methylphenyl)methylene]-				
Synonyms					
CAS No	36861-47-9		EINECS No	253-242-6	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.92	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.008				ECOSAR
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity				
Water solubility (mg/l)	0.2			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	Web has use as UV absorber in cosmetics				
Potential for exposure over wide scale?	Yes, based on confidential use information and on web information				
Overall comments	High priority for further investigation (also identified in UV filter review)				

Project code no.	PvB93				
Substance name	Benzene, pentabromo(bromomethyl)-				
Synonyms					
CAS No	38521-51-6	EINECS No		253-985-6	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.33	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	No predicted value				ECOSAR
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity				
Water solubility (mg/l)	0.0001			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB [EA (2003) concludes PBT]				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has use as reactive flame retardant				
Potential for exposure over wide scale?	No, based on confidential use information and *Kirk-Othmer* information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB95				
Substance name	Benzene, 1,4-dichloro-2,5-bis(dichloromethyl)-				
Synonyms					
CAS No	41999-84-2	EINECS No	255-618-5		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.25	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	No predicted value				ECOSAR
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity				
Water solubility (mg/l)	0.34			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB96				
Substance name	Cyclopropanecarboxylic acid, 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester				
Synonyms	Cyhalothrin				
CAS No	68085-85-8		EINECS No	268-450-2	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.85	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.003				ECOSAR
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity				
Water solubility (mg/l)	0.0008			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	*Kirk-Othmer* and web information have use as insecticide				
Potential for exposure over wide scale?	Yes, based on confidential use information, and on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB97				
Substance name	Peroxide, (1,1,4,4-tetramethyl-2-butyne-1,4-diyl)bis[(1,1-dimethylethyl)				
Synonyms					
CAS No	1068-27-5		EINECS No	213-944-5	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.84	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	No predicted value				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.15			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	Web and *Kirk-Othmer* have use as polymer cross-linking agent				
Potential for exposure over wide scale?	No, based on confidential use information and *Kirk-Othmer* and web information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB98				
Substance name	2-Naphthalenecarboxamide, N-[4-(acetylamino)phenyl]-4-[[5-(aminocarbonyl)-2-chlorophenyl]azo]-3-hydroxy-				
Synonyms					
CAS No	12236-64-5	EINECS No		235-464-5	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.79	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.012				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.01			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB99				
Substance name	Acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-ethoxyphenyl]-				
Synonyms					
CAS No	12239-34-8	EINECS No		235-475-5	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.53	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.004				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.0009 (measured)			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	*Kirk-Othmer* and web have use as dye.				
Potential for exposure over wide scale?	Yes, based on confidential use information and on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB100				
Substance name	2-Naphthalenol, 1-[(2-methoxyphenyl)azo]-				
Synonyms					
CAS No	1229-55-6	EINECS No		214-968-9	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.59	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.008				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.0003 (measured)			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* and web have use as colourant for plastics				
Potential for exposure over wide scale?	Yes, based on confidential use information, and on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB101				
Substance name	Benzo[b]thiophen-3(2H)-one, 4,7-dichloro-2-(4,7-dichloro-3-oxobenzo[b]thien-2(3H)-ylidene)-				
Synonyms					
CAS No	14295-43-3		EINECS No	238-222-7	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.11	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.01				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.01			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has use as a colourant for plastics				
Potential for exposure over wide scale?	Yes, based on confidential use information and on *Kirk-Othmer* information				
Overall comments	High priority for further investigation				

Project code no.	PvB102				
Substance name	Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 2',4',5',7'-tetrabromo-3',6'-dihydroxy-				
Synonyms					
CAS No	15086-94-9		EINECS No	239-138-3	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.91	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.005				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.00003			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	Web has use as dye				
Potential for exposure over wide scale?	Yes, based on web information				
Overall comments	High priority for further investigation				

Project code no.	PvB103				
Substance name	9,10-Anthracenedione, 1-[[4-(phenylsulfonyl)phenyl]amino]-				
Synonyms					
CAS No	15958-61-9		EINECS No	240-092-1	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.36	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.007				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.0005			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB104				
Substance name	Ethanol, 2,2'-[[4-[(2-bromo-6-chloro-4-nitrophenyl)azo]-3-chlorophenyl]imino]bis-				
Synonyms					
CAS No	17464-91-4	EINECS No		241-481-9	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.32	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.059				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.01			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB105				
Substance name	Phenol, 4-[[2-methoxy-4-[(4-nitrophenyl)azo]phenyl]azo]-				
Synonyms					
CAS No	19800-42-1		EINECS No	243-325-5	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.23	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.006				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.03			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* and web have use as dye				
Potential for exposure over wide scale?	Yes, based on confidential use information, and on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB106				
Substance name	9,10-Anthracenedione, 1,8-dihydroxy-4-nitro-5-(phenylamino)-				
Synonyms					
CAS No	20241-76-3		EINECS No	243-632-4	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.38	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.005				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.004			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	*Kirk-Othmer* and web have use as dye				
Potential for exposure over wide scale?	Yes, based on confidential use information, and on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB107				
Substance name	Ethanol, 2,2'-[[3-chloro-4-[(2,6-dichloro-4-nitrophenyl)azo]phenyl]imino]bis-				
Synonyms					
CAS No	23355-64-8		EINECS No	245-604-7	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.08	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.087				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.03			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB108				
Substance name	2-Naphthalenol, 1-[(4-methyl-2-nitrophenyl)azo]-				
Synonyms					
CAS No	2425-85-6	EINECS No	219-372-2		
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	6.45	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF	<2.9	BCF data type	Measured	BCF source	CHRIP
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.004				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.05			WS source	EPI SUITE
P classification	P (provisional)				
B classification	Not B (based on measured result accepted by regulatory authority)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Not PBT				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* and web have use as a pigment				
Potential for exposure over wide scale?	Yes, based on confidential use information, and on *Kirk-Othmer* and web information				
Overall comments	Low priority for further investigation				

Project code no.	PvB109				
Substance name	Benzonitrile, 2-[[4-[(2-cyanoethyl)(2-phenylethyl)amino]phenyl]azo]-5-nitro-				
Synonyms					
CAS No	24610-00-2		EINECS No	246-352-0	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.94	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.015				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.004			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB110				
Substance name	Peroxide, [1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[(1,1-dimethylethyl)				
Synonyms					
CAS No	25155-25-3		EINECS No	246-678-3	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL, OECD HPV				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.34	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	No predicted value				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.004			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* and web have use as cross-linking agent in polymers				
Potential for exposure over wide scale?	No, based on confidential use information, and on *Kirk-Othmer* and web information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB111				
Substance name	2-Naphthalenol, 1-[(2-chloro-4-nitrophenyl)azo]-				
Synonyms					
CAS No	2814-77-9	EINECS No		220-562-2	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.55	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.004				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.03			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* and web have use as pigment				
Potential for exposure over wide scale?	Yes, based on confidential use information, and on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB112				
Substance name	2-Naphthalenol, 1-[(2,4-dinitrophenyl)azo]-				
Synonyms					
CAS No	3468-63-1	EINECS No		222-429-4	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.72	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00174				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.13			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB113				
Substance name	Nickel, bis[2,3-bis(hydroxyimino)-N-(2-methoxyphenyl)butanamidato]-				
Synonyms					
CAS No	42739-61-7		EINECS No	255-924-9	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.58	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.142				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.0007			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB114				
Substance name	Benzenesulfonic acid, 4-[[3-[[2-hydroxy-3-[[(4-methoxyphenyl)amino]carbonyl]-1-naphthalenyl]azo]-4-methylbenzoyl]amino]-, calcium salt (2:1)				
Synonyms					
CAS No	43035-18-3	EINECS No		256-050-0	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.46	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.003				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.00004			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB115				
Substance name	Benzo[h]benz[5,6]acridino[2,1,9,8-klmna]acridine-8,16-dione				
Synonyms					
CAS No	475-71-8	EINECS No		207-498-0	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.0	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.013				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.002			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* and web have use as dye				
Potential for exposure over wide scale?	Yes, based on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB116				
Substance name	Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-bis(diethylamino)-				
Synonyms					
CAS No	509-34-2		EINECS No	208-096-8	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	6.63	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.004				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.0003			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, on web				
Summary of use	*Kirk-Othmer* and web have use as dye				
Potential for exposure over wide scale?	Yes, based on confidential use information, and on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB117				
Substance name	Propanenitrile, 3-[[2-(acetyloxy)ethyl][4-[(2,6-dichloro-4-nitrophenyl)azo]phenyl]amino]-				
Synonyms					
CAS No	5261-31-4	EINECS No		226-070-4	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.52	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.032				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.005			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	*Kirk-Othmer* and web have use as dye				
Potential for exposure over wide scale?	Yes, based on confidential use information, and on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB118				
Substance name	Acetamide, N-[2-[(2-bromo-4,6-dinitrophenyl)azo]-5-(diethylamino)phenyl]-				
Synonyms					
CAS No	52697-38-8		EINECS No	258-110-1	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.88	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.002				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.003			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	Web has use as dye				
Potential for exposure over wide scale?	Yes, based on confidential use information and on web information				
Overall comments	High priority for further investigation				

Project code no.	PvB119				
Substance name	Phosphorous acid, (1-methylethylidene)di-4,1-phenylene tetrakis[(3-ethyl-3-oxetanyl)methyl] ester				
Synonyms					
CAS No	53184-75-1		EINECS No	258-419-1	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.96	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.000467				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.000003			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB121				
Substance name	2-Naphthalenecarboxamide, 4-[[5-[[[4-(aminocarbonyl)phenyl]amino]carbonyl]-2-methoxyphenyl]azo]-N-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxy-				
Synonyms					
CAS No	59487-23-9	EINECS No	261-785-5		
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.07	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.004				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.00009			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	Web has use as pigment				
Potential for exposure over wide scale?	Yes, based on confidential use information and on web information				
Overall comments	High priority for further investigation				

Project code no.	PvB122				
Substance name	Pyridinium, 1-[2-[[4-[(2-chloro-4-nitrophenyl)azo]phenyl]ethylamino]ethyl]-, acetate				
Synonyms					
CAS No	59709-10-3		EINECS No	261-873-3	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.83	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.002				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.001			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB123				
Substance name	β-Alanine, N-[4-[(2-bromo-6-chloro-4-nitrophenyl)azo]phenyl]-N-(3-methoxy-3-oxopropyl)-, methyl ester				
Synonyms					
CAS No	59709-38-5		EINECS No	261-874-9	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.28	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.009				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.0008			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB124				
Substance name	Phenol, 4-[[4-(phenylazo)phenyl]azo]-				
Synonyms					
CAS No	6250-23-3	EINECS No		228-370-0	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.75	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.008				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.00006 (measured)			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	*Kirk-Othmer* has use as colourant for plastics				
Potential for exposure over wide scale?	Yes, based on confidential use information and on *Kirk-Othmer* information				
Overall comments	High priority for further investigation				

Project code no.	PvB125				
Substance name	3H-Pyrazol-3-one, 4-[(2,4-dimethylphenyl)azo]-2,4-dihydro-5-methyl-2-phenyl-				
Synonyms					
CAS No	6407-78-9		EINECS No	229-043-5	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.65	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.003				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.06			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	Web has use as a colourant				
Potential for exposure over wide scale?	Yes, based on confidential use information and on web information				
Overall comments	High priority for further investigation				

Project code no.	PvB126				
Substance name	2-Naphthalenecarboxamide, N-(5-chloro-2,4-dimethoxyphenyl)-4-[[5-[(diethylamino)sulfonyl]-2-methoxyphenyl]azo]-3-hydroxy-				
Synonyms					
CAS No	6410-41-9	EINECS No		229-107-2	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.65	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.002				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.00004			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* and web have use as pigment				
Potential for exposure over wide scale?	Yes, based on confidential use information, and on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB127				
Substance name	7-Oxa-3,20-diazadispiro[5.1.11.2]heneicosan-21-one, 2,2,4,4-tetramethyl-				
Synonyms					
CAS No	64338-16-5		EINECS No	264-780-6	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.39	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.107				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.02			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	Web has use as a light stabiliser and pigment				
Potential for exposure over wide scale?	Yes, based on confidential use information and on web information				
Overall comments	High priority for further investigation				

Project code no.	PvB128				
Substance name	Phosphonic acid, [[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-, monoethyl ester, calcium salt (2:1)				
Synonyms					
CAS No	65140-91-2		EINECS No	265-512-0	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.08	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.0102				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.0009			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* and web have use as anti-oxidant				
Potential for exposure over wide scale?	Yes, based on confidential use information, and on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB129				
Substance name	Peroxide, (3,3,5-trimethylcyclohexylidene)bis[(1,1-dimethylethyl)				
Synonyms					
CAS No	6731-36-8	EINECS No	229-782-3		
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	7.56	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF	13,200	BCF data type	Measured	BCF source	CHRIP
Lowest acute ecotox L(E)C50 (mg/l)	0.006			Ecotox source	ECOSAR
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.004			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (based on measured result accepted by regulatory authority; EURAS gold-standard database has similar value)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has use as cross-linking agent				
Potential for exposure over wide scale?	No, based on confidential use information and on *Kirk-Othmer* information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB130				
Substance name	1-Naphthalenemethanol, α,α-bis[4-(dimethylamino)phenyl]-4-(phenylamino)-				
Synonyms					
CAS No	6786-83-0		EINECS No	229-851-8	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.21	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	5×10^{-6}			Ecotox source	ECOSAR
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.0006			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	Web has use as colourant				
Potential for exposure over wide scale?	Yes, based on confidential use information and on web information				
Overall comments	High priority for further investigation				

Project code no.	PvB131				
Substance name	Alcohols, C8–14, γ-ω-perfluoro				
Synonyms					
CAS No	68391-08-2	EINECS No		269-927-8	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.44	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.035				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.4			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	Web indicates use as raw material for low surface tension coatings				
Potential for exposure over wide scale?	No, based on confidential use information and on web information				
Overall comments	Medium priority for further investigation; log K_{ow} may be unreliable as an indicator of bioaccumulation potential for this type of substance				

Project code no.	PvB132				
Substance name	Acetamide, N-[2-[(2-bromo-4,6-dinitrophenyl)azo]-5-[(2-cyanoethyl)-2-propenylamino]-4-methoxyphenyl]-				
Synonyms					
CAS No	68877-63-4	EINECS No		272-569-5	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.34	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.004				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.0007 (measured)			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB133				
Substance name	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, (1,2-dioxo-1,2-ethanediyl)bis(imino-2,1-ethanediyl) ester				
Synonyms					
CAS No	70331-94-1	EINECS No		274-572-7	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.92	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00188				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.00002			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has use as anti-oxidant				
Potential for exposure over wide scale?	Yes, based on *Kirk-Othmer* use information				
Overall comments	High priority for further investigation				

Project code no.	PvB134				
Substance name	1-Naphthalenamine, 4-[(2-bromo-4,6-dinitrophenyl)azo]-N-(3-methoxypropyl)-				
Synonyms					
CAS No	70660-55-8		EINECS No	274-733-1	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.24	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00156				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.001			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB135				
Substance name	Chromate(1-), bis[3,5-bis(1,1-dimethylethyl)-2-hydroxybenzoato(2-)-O1,O2]-, hydrogen				
Synonyms					
CAS No	72869-85-3		EINECS No	276-955-4	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.92	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.003				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.0004			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB136				
Substance name	Methanesulfonamide, N-[2-[(2,6-dicyano-4-methylphenyl)azo]-5-(dipropylamino)phenyl]-				
Synonyms					
CAS No	72968-82-2		EINECS No	277-156-3	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.09	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.086				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.02			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB137				
Substance name	9,10-Anthracenedione, 1-[(5,7-dichloro-1,9-dihydro-2-methyl-9-oxopyrazolo[5,1-b]quinazolin-3-yl)azo]-				
Synonyms					
CAS No	74336-60-0	EINECS No		277-824-4	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.68	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.005				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.0003			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information and no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB138				
Substance name	Peroxide, (1,1,4,4-tetramethyl-1,4-butanediyl)bis[(1,1-dimethylethyl)				
Synonyms					
CAS No	78-63-7	EINECS No	201-128-1		
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	6.55	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF	3690	BCF data type	Measured	BCF source	CHRIP
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	No predicted value				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.04			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (based on measured result accepted by regulatory authority)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has use as cross-linking agent				
Potential for exposure over wide scale?	No, based on confidential use information and *Kirk-Othmer* information				
Overall comments	Medium priority for further investigation				

Project code no.	PvB139				
Substance name	Benzenesulfonic acid, 2,2'-[(9,10-dihydro-5,8-dihydroxy-9,10-dioxo-1,4-anthracenediyl)diimino]bis[5-(1,1-dimethylethyl)-, disodium salt				
Synonyms					
CAS No	83006-67-1		EINECS No	280-116-8	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.32	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.006				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.0002			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB140				
Substance name	3H-Indol-3-one, 5,7-dibromo-2-(5-bromo-7-chloro-1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-				
Synonyms					
CAS No	85702-64-3	EINECS No	288-256-1		
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	6.43	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.007				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.001			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PvB141				
Substance name	2-Naphthalenol, 1-[[4-(phenylazo)phenyl]azo]-				
Synonyms					
CAS No	85-86-9	EINECS No		201-638-4	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	7.63	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00128				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.002			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* and web have use as colourant				
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PvB142				
Substance name	2-Naphthalenol, 1-(phenylazo)-				
Synonyms					
CAS No	842-07-9	EINECS No		212-668-2	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	5.51	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	2.5×10^{-6}				ECOSAR
Ecotoxicity comments					
Water solubility (mg/l)	0.7			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB. Note T based on inclusion on Canadian PBiThuman list				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	*Kirk-Othmer* and web sites have use as a dye				
Potential for exposure over wide scale?	Yes, based on confidential use information, and on *Kirk-Othmer* and web information				
Overall comments	High priority for further investigation				

Project code no.	PvB143				
Substance name	Colecalciferol, Vitamin D3				
Synonyms	9,10-Secocholesta-5,7,10(19)-trien-3-ol, (3-beta,5Z,7E)-				
CAS No	67-97-0	EINECS No	200-673-2		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	10.24	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	2.5×10^{-6}				ECOSAR
Ecotoxicity comments					
Water solubility (mg/l)	2×10^{-5}			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB. T based on Annex 1 classification with R48.				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has food additive				
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	Low priority for further investigation as naturally occurring food component.				

Project code no.	PvB144				
Substance name	1-(5,6,7,8-Tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthyl)ethan-1-one				
Synonyms					
CAS No	21145-77-7		EINECS No	244-240-6	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (report screening)			Biodegradation source	EA (in prep.)
Biodegradation comments					
Log K_{ow}	5.7	K_{ow} data type	Measured	Log K_{ow} source	EA (in prep.)
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.023			Ecotox source	EA (in prep.)
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments					
Water solubility (mg/l)	1.25 (measured)			WS source	EA (in prep.)
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	EA (in prep.) has use in fragrances				
Potential for exposure over wide scale?	Yes, based on EA (in prep.)				
Overall comments	This is an alternative CAS no. for the substance AHTN (CAS no. 1506-02-1), which has been assessed by the EU PBT WG and concluded not to have PBT properties; low priority for further investigation				

Project code no.	PvB145				
Substance name	2-Ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol				
Synonyms					
CAS No	28219-61-6		EINECS No	248-908-8	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (report screening)			Biodegradation source	EA (in prep.)
Biodegradation comments					
Log K_{ow}	5.14	K_{ow} data type	Predicted	Log K_{ow} source	EA (in prep.)
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.23			Ecotox source	EA (in prep.)
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	Narrowly fails to meet the screening T criterion				
Water solubility (mg/l)	5.2			WS source	EA (in prep.)
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	EA (in prep.) has use in fragrances				
Potential for exposure over wide scale?	Yes, based on EA (in prep.)				
Overall comments	High priority for further investigation				

Project code no.	PvB146				
Substance name	Methyl 2,6,10-trimethylcyclododeca-2,5,9-trien-1-yl ketone				
Synonyms					
CAS No	28371-99-5		EINECS No	248-995-2	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (report screening)			Biodegradation source	EA (in prep.)
Biodegradation comments					
Log K_{ow}	5.98	K_{ow} data type	Predicted	Log K_{ow} source	EA (in prep.)
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.047			Ecotox source	EA (in prep.)
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments					
Water solubility (mg/l)	0.19			WS source	EA (in prep.)
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	EA (in prep.) has use in fragrances				
Potential for exposure over wide scale?	Yes, based on EA (in prep.)				
Overall comments	High priority for further investigation				

Project code no.	PvB147				
Substance name	6-Tert-butyl-1,1-dimethylindan-4-yl methyl ketone				
Synonyms	Celestolide				
CAS No	13171-00-1		EINECS No	236-114-4	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EA (in prep.)
Biodegradation comments					
Log K_{ow}	6.02	K_{ow} data type	Predicted	Log K_{ow} source	EA (in prep.)
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.05			Ecotox source	EA (in prep.)
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments					
Water solubility (mg/l)	0.22			WS source	EA (in prep.)
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	EA (in prep.) has use in fragrances				
Potential for exposure over wide scale?	Yes, based on EA (in prep.)				
Overall comments	High priority for further investigation				

Project code no.	PvB148				
Substance name	Caryophyllene				
Synonyms					
CAS No	87-44-5		EINECS No	201-746-1	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (report screening)			Biodegradation source	EA (in prep.)
Biodegradation comments					
Log K_{ow}	6.3	K_{ow} data type	Predicted	Log K_{ow} source	EA (in prep.)
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.02			Ecotox source	EA (in prep.)
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments					
Water solubility (mg/l)	0.05			WS source	EA (in prep.)
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	EA (in prep.) has use in fragrances				
Potential for exposure over wide scale?	Yes, based on EA (in prep.)				
Overall comments	High priority for further investigation				

Project code no.	PvB149				
Substance name	a,b,2,2,3-Pentamethylcyclopent-3-ene-1-butanol				
Synonyms					
CAS No	65113-99-7		EINECS No	265-453-0	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (report screening)			Biodegradation source	EA (in prep.)
Biodegradation comments					
Log K_{ow}	5.15	K_{ow} data type	Predicted	Log K_{ow} source	EA (in prep.)
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.23			Ecotox source	EA (in prep.)
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	Narrowly fails to meet the screening T criterion				
Water solubility (mg/l)	5.0			WS source	EA (in prep.)
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	EA (in prep.) has use in fragrances				
Potential for exposure over wide scale?	Yes, based on EA (in prep.)				
Overall comments	High priority for further investigation				

Project code no.	PvB150				
Substance name	[3R-(3a,3ab,6a,7b,8aa)]-Octahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl acetate				
Synonyms	Cedryl acetate				
CAS No	77-54-3		EINECS No	201-036-1	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (report) screening)			Biodegradation source	EA (in prep.)
Biodegradation comments					
Log K_{ow}	5.33	K_{ow} data type	Predicted	Log K_{ow} source	EA (in prep.)
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.2			Ecotox source	EA (in prep.)
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	Narrowly fails to meet the screening T criterion				
Water solubility (mg/l)	0.55			WS source	EA (in prep.)
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	EA (in prep.) has use in fragrances				
Potential for exposure over wide scale?	Yes, based on EA (in prep.)				
Overall comments	High priority for further investigation				

Project code no.	PvB151				
Substance name	4,4'-Thio-bis(2-t-butyl-5-methylphenol)				
Synonyms					
CAS No	96-69-5	EINECS No	202-525-2		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP, US HPV
Biodegradation (predicted)	Not readily biodegradable (report screening)			Biodegradation source	EA (2003)
Biodegradation comments					
Log K_{ow}	8.24	K_{ow} data type	Predicted	Log K_{ow} source	EA (2003)
BCF	11	BCF data type	Measured	BCF source	CHRIP
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.054 (measured)				US HPV
Ecotoxicity comments	T based on EA (2003) assessment				
Water solubility (mg/l)	0.1			WS source	US HPV
P classification	P (provisional)				
B classification	Not B (based on measured result accepted by regulatory authority)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Not PBT				
Possible UK suppliers (with source)					
Summary of use	EA (2003) has use as flame retardant				
Potential for exposure over wide scale?	Yes, based on EA (2003)				
Overall comments	Low priority for further investigation; previously flagged as potential PBT in EA (2003)				

Project code no.	PvB152				
Substance name	Dodecachlorodimethan-o-dibenzocyclooctane				
Synonyms	Dechlorane® Plus				
CAS No	13560-89-9	EINECS No	236-948-9		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	US HPV, CHRIP
Biodegradation (predicted)	Not readily biodegradable (report screening)			Biodegradation source	EA (2003)
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	11.27	K_{ow} data type	Predicted	Log K_{ow} source	EA (2003)
BCF	121	BCF data type	Measured	BCF source	CHRIP, EURAS
Lowest acute ecotox L(E)C50 (mg/l)	No effects at solubility			Ecotox source	US HPV
Lowest chronic ecotox NOEC (mg/l)	No effects at solubility				CHRIP
Ecotoxicity comments	T originally based on EA (2003) assessment, experimental data indicates not T				
Water solubility (mg/l)	0.25			WS source	US HPV
P classification	P (provisional)				
B classification	Not B (based on measured result accepted by regulatory authority and included in gold-standard database)				
T classification – aquatic only	Not T	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Not PBT				
Possible UK suppliers (with source)					
Summary of use	EA (2003) has use as flame retardant				
Potential for exposure over wide scale?	Yes, based on EA (2003)				
Overall comments	Low priority for further investigation; previously flagged as potential PBT in EA (2003)				

Project code no.	PvB153				
Substance name	Tetrabromobisphenol-A bis(allylether)				
Synonyms					
CAS No	25327-89-3		EINECS No	246-850-8	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (report screening)			Biodegradation source	EA (2003)
Biodegradation comments					
Log K_{ow}	10.02	K_{ow} data type	Predicted	Log K_{ow} source	EA (2003)
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	6×10^{-5}				ECOSAR
Ecotoxicity comments	T based on EA (2003) assessment				
Water solubility (mg/l)	1×10^{-6}			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	EA (2003) has use as reactive flame retardant				
Potential for exposure over wide scale?	No, based on EA (2003)				
Overall comments	Medium priority for further investigation				

Project code no.	PvB154				
Substance name	Phthalic acid, tetrabromo-, bis(2-ethylhexyl) ester				
Synonyms	Tetrabromophthalic acid, diethylhexyl ester				
CAS No	26040-51-7	EINECS No	247-426-5		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	US HPV
Biodegradation (predicted)	Not readily biodegradable (report screening)			Biodegradation source	EA (2003)
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	11.95	K_{ow} data type	Predicted	Log K_{ow} source	EA (2003)
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.38 (measured)			Ecotox source	US HPV
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	T based on EA (2003) assessment				
Water solubility (mg/l)	<0.001			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	EA (2003) has use as flame retardant				
Potential for exposure over wide scale?	Yes, based on EA (2003)				
Overall comments	High priority for further investigation; this substance is a brominated analogue of di(ethylhexyl)phthalate (DEHP), a Category 2 reprotoxin				

Project code no.	PvB155				
Substance name	Tetradecabromodiphenoxybenzene				
Synonyms					
CAS No	58965-66-5	EINECS No		261-526-6	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (report screening)			Biodegradation source	EA (2003)
Biodegradation comments					
Log K_{ow}	16.89	K_{ow} data type	Predicted	Log K_{ow} source	EA (2003)
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	1×10^{-11}				ECOSAR
Ecotoxicity comments	T based on EA (2003) assessment				
Water solubility (mg/l)	$<1 \times 10^{-6}$			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	EA (2003) has use as additive flame retardant				
Potential for exposure over wide scale?	Yes, based on EA (2003)				
Overall comments	High priority for further investigation				

Project code no.	PvB156				
Substance name	Homosalate				
Synonyms	Homomenthyl salicylate; 3,3,5-trimethylcyclohexyl salicylate				
CAS No	118-56-9	EINECS No	204-260-8		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (report screening)			Biodegradation source	EA (2008)
Biodegradation comments					
Log K_{ow}	6.16	K_{ow} data type	Predicted	Log K_{ow} source	EA (2008)
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.005				EA (2008)
Ecotoxicity comments	T based on EA (2008) assessment				
Water solubility (mg/l)	0.42			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	EA (2008) has use as UV filter in cosmetics				
Potential for exposure over wide scale?	Yes, based on EA (2008)				
Overall comments	High priority for further investigation				

Project code no.	PvB157				
Substance name	Ethylhexyl dimethyl dimethyl-*p*-aminobenzoate [ethylhexyl dimethyl PABA]				
Synonyms	2-Ethylhexyl 4-dimethylaminobenzoate; octyldimethyl PABA				
CAS No	21245-02-3		EINECS No	244-289-3	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (report screening)			Biodegradation source	EA (2008)
Biodegradation comments					
Log K_{ow}	5.77	K_{ow} data type	Predicted	Log K_{ow} source	EA (2008)
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.012				EA (2008)
Ecotoxicity comments	T based on EA (2008) assessment				
Water solubility (mg/l)	0.2			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	EA (2008) has use as UV filter in cosmetics				
Potential for exposure over wide scale?	Yes, based on EA (2008)				
Overall comments	High priority for further investigation				

Project code no.	PvB158				
Substance name	Octocrylene				
Synonyms	2-Ethylhexyl 2-cyano-3,3-diphenylacrylate				
CAS No	6197-30-4	EINECS No		228-250-8	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (report screening)			Biodegradation source	EA (2008)
Biodegradation comments					
Log K_{ow}	6.38	K_{ow} data type	Predicted	Log K_{ow} source	EA (2008)
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00089				EA (2008)
Ecotoxicity comments	T based on EA (2008) assessment				
Water solubility (mg/l)	0.004			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use	EA (2008) has use as UV filter in cosmetics				
Potential for exposure over wide scale?	Yes, based on EA (2008)				
Overall comments	High priority for further investigation				

Project code no.	PvB159				
Substance name	3-Benzylidene camphor				
Synonyms					
CAS No	15087-24-8		EINECS No	239-139-9	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (report screening)			Biodegradation source	EA (2008)
Biodegradation comments					
Log K_{ow}	5.37	K_{ow} data type	Predicted	Log K_{ow} source	EA (2008)
BCF	493	BCF data type	Measured	BCF source	EURAS
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.022				EA (2008)
Ecotoxicity comments	T based on EA (2008) assessment as possible endocrine-disrupting chemical				
Water solubility (mg/l)	0.7			WS source	EPI SUITE
P classification	P (provisional)				
B classification	Not B (based on value from EURAS BCF gold-standard database)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Not PBT				
Possible UK suppliers (with source)					
Summary of use	EA (2008) has use as UV filter in cosmetics				
Potential for exposure over wide scale?	Yes, based on EA (2008)				
Overall comments	Low priority on basis of PBT properties, though high priority for further investigation as possible endocrine-disrupting chemical				

Project code no.	PB1				
Substance name	D-Glucofuranoside, ethyl 3,5,6-tris-O-(phenylmethyl)-				
Synonyms					
CAS No	10310-32-4		EINECS No	233-687-2	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.94	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.127				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.19			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	Web information has use as pharmaceutical intermediate				
Potential for exposure over wide scale?	No, based on confidential use information and on web information				
Overall comments	Medium priority for further investigation				

Project code no.	PB2				
Substance name	Benzenemethanamine, N-ethyl-N-(3-methylphenyl)-				
Synonyms					
CAS No	119-94-8	EINECS No	204-359-6		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.62	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.113				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	3.68			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PB3				
Substance name	Pyrene				
Synonyms					
CAS No	129-00-0		EINECS No	204-927-3	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.93	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF	53	BCF data type	Measured	BCF source	EURAS
Lowest acute ecotox L(E)C50 (mg/l)	1.0			Ecotox source	CHRIP
Lowest chronic ecotox NOEC (mg/l)	0.005				CHRIP
Ecotoxicity comments	T from Danish EPA predictions and based on measured result accepted by regulatory authority				
Water solubility (mg/l)	0.14 (measured)			WS source	EPI SUITE
P classification	P (provisional)				
B classification	Not B (based on value from EURAS BCF gold-standard database)				
T classification – aquatic only	T	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	See overall comments				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	This substance is a component of various coal-tar products, some of which have been considered for identification as Substances of Very High Concern under REACH already. For example, the dossier for 'coal tar pitch – high temperature' (CAS no. 65996-93-2) indicates that pyrene should be considered a PBT/vPvB substance on the basis of additional BCF data. It is therefore a low priority for further investigation for the purposes of this project.				

Project code no.	PB4				
Substance name	Benzoic acid, 2-hydroxy-3,5-diiodo-				
Synonyms					
CAS No	133-91-5		EINECS No	205-124-0	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.58	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.327				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	1.71			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PB5				
Substance name	Benzenamine, 2,6-dichloro-N-phenyl-				
Synonyms					
CAS No	15307-93-4		EINECS No	239-349-0	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.58	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.129				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	3.37			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PB6				
Substance name	Phenol, 5-chloro-2-(2,4-dichlorophenoxy)-				
Synonyms					
CAS No	3380-34-5	EINECS No	222-182-2		
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.66 4.75	K_{ow} data type	Predicted Measured	Log K_{ow} source	EPI SUITE CHRIP
BCF	90	BCF data type	Measured	BCF source	CHRIP, EURAS
Lowest acute ecotox L(E)C50 (mg/l)	0.002			Ecotox source	CHRIP
Lowest chronic ecotox NOEC (mg/l)	0.00034				CHRIP
Ecotoxicity comments	T from Danish EPA predictions and based on measured result accepted by regulatory authority				
Water solubility (mg/l)	100			WS source	CHRIP
P classification	P (provisional)				
B classification	Not B (based on measured result accepted by regulatory authority and on value from EURAS BCF gold-standard database)				
T classification – aquatic only	T	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Not PBT				
Possible UK suppliers (with source)					
Summary of use	Web information has use as anti-microbial agent				
Potential for exposure over wide scale?	Yes, based on web information				
Overall comments	Low priority for further investigation				

Project code no.	PB7				
Substance name	1,1'-Biphenyl, 4-bromo-2-fluoro-				
Synonyms					
CAS No	41604-19-7		EINECS No	255-453-9	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.85	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.079				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	1.69			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PB8				
Substance name	2-Naphthalenecarboxamide, N-(4-chloro-2,5-dimethoxyphenyl)-3-hydroxy-				
Synonyms					
CAS No	4273-92-1	EINECS No		224-270-6	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.72	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.026				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	1.98			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)					
Summary of use	Web information has use as pigment intermediate				
Potential for exposure over wide scale?	No, based on confidential use information and on web information				
Overall comments	Medium priority for further investigation				

Project code no.	PB9				
Substance name	1-Butanone, 4-chloro-1-[4-(1,1-dimethylethyl)phenyl]-				
Synonyms					
CAS No	43076-61-5		EINECS No	256-077-8	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.82	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	No predicted value				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	2.1			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PB10				
Substance name	Bicyclo[2.2.1]heptane, 2-chloro-1,7,7-trimethyl-, endo-				
Synonyms					
CAS No	464-41-5		EINECS No	207-350-5	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.57	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.096				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	7.46			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PB11				
Substance name	Benzenemethanol, 4-(dimethylamino)-alpha,alpha-bis[4-(dimethylamino)phenyl]-				
Synonyms					
CAS No	467-63-0	EINECS No		207-396-6	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.91	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.00067			Ecotox source	ECOSAR
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	T from Danish EPA predictions				
Water solubility (mg/l)	0.22			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	Web information has use as a dye				
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PB12				
Substance name	Benzamide, 5-chloro-N-(2-chloro-4-nitrophenyl)-2-hydroxy-				
Synonyms					
CAS No	50-65-7		EINECS No	200-056-8	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.56	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.028				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	1.68			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* and web information have use as anthelmintic, against tapeworms in animals				
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PB13				
Substance name	1,3-Benzodioxole, 5-[[2-(2-butoxyethoxy)ethoxy]methyl]-6-propyl-				
Synonyms					
CAS No	51-03-6	EINECS No		200-076-7	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.29	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.329				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	14.3			WS source	CHRIP
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)	Yes, on web				
Summary of use	*Kirk-Othmer* has use as insecticide				
Potential for exposure over wide scale?	Yes, based on confidential use information and on *Kirk-Othmer* information				
Overall comments	High priority for further investigation				

Project code no.	PB14				
Substance name	Phosphorothioic acid, O-(2,6-dichloro-4-methylphenyl) O,O-dimethyl ester				
Synonyms					
CAS No	57018-04-9		EINECS No	260-515-3	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.77	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.089				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	1.1 (measured)			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	Pesticide				
Potential for exposure over wide scale?	Yes, based on use information				
Overall comments	High priority for further investigation				

Project code no.	PB15				
Substance name	Benzene, 1,3,5-tribromo-				
Synonyms					
CAS No	626-39-1	EINECS No		210-947-3	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.66	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF	5000	BCF data type	Measured	BCF source	EURAS
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.146				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.79 (measured)			WS source	EPI SUITE
P classification	P (provisional)				
B classification	vB (provisional) (based on value from EURAS BCF gold-standard database)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT, vPvB				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PB16				
Substance name	Benzene, 1,2,3,4-tetrachloro-				
Synonyms					
CAS No	634-66-2		EINECS No	211-214-0	
Existing regulatory and related activity (e.g. priority lists)	OSPAR, Canadian DSL				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	4.57 4.55	K_{ow} data type	Predicted Measured	Log K_{ow} source	EPI SUITE CHRIP
BCF	1710	BCF data type	Measured	BCF source	CHRIP, EURAS
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.12				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.433			WS source	CHRIP
P classification	P (provisional)				
B classification	Narrowly misses B (based on measured result accepted by regulatory authority and on value from EURAS BCF gold-standard database)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)	Yes, on web				
Summary of use	Web information has use as intermediate				
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PB17				
Substance name	Benzoic acid, 3-[2-chloro-4-(trifluoromethyl)phenoxy]-				
Synonyms					
CAS No	63734-62-3		EINECS No	264-433-9	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.7	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	2.6			Ecotox source	US HPV
Lowest chronic ecotox NOEC (mg/l)	1.354				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.95			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	No, based on confidential use information				
Overall comments	Medium priority for further investigation				

Project code no.	PB18				
Substance name	Urea, N-[(4-chlorophenyl)methyl]-N-cyclopentyl-N'-phenyl-				
Synonyms					
CAS No	66063-05-6		EINECS No	266-096-3	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.82	K_{ow} data type	Measured	Log K_{ow} source	Danish EPA
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.028				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.3 (measured)			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)					
Summary of use	Web information has use as fungicide				
Potential for exposure over wide scale?	Yes, based on confidential use information and on web information				
Overall comments	High priority for further investigation				

Project code no.	PB19				
Substance name	Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-, (1R)-				
Synonyms					
CAS No	7785-70-8		EINECS No	232-087-8	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.27	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.138				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	2.49 (measured)			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)					
Summary of use	Web has use as intermediate in organic synthesis				
Potential for exposure over wide scale?	No, based on web information				
Overall comments	Medium priority for further investigation				

Project code no.	PB20				
Substance name	7H-Benz[de]anthracen-7-one				
Synonyms					
CAS No	82-05-3	EINECS No	201-393-3		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.73 4.81	K_{ow} data type	Predicted Measured	Log K_{ow} source	EPI SUITE CHRIP
BCF	181	BCF data type	Measured	BCF source	CHRIP, EURAS
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.093				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.18			WS source	EPI SUITE
P classification	P (provisional)				
B classification	Not B (based on measured result accepted by regulatory authority and on value from EURAS BCF gold-standard database)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Not PBT				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	*Kirk-Othmer* has use as intermediate for vat dyes				
Potential for exposure over wide scale?	No, based on confidential use information and *Kirk-Othmer* information				
Overall comments	Low priority for further investigation				

Project code no.	PB22				
Substance name	2-Naphthalenecarboxamide, N-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxy-				
Synonyms					
CAS No	92-72-8	EINECS No		202-182-9	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.72	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.026				ECOSAR
Ecotoxicity comments	T from Danish EPA predictions (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	1.98			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has use in pigments, web information has use as dye intermediate				
Potential for exposure over wide scale?	Yes, based on *Kirk-Othmer* information				
Overall comments	High priority for further investigation				

Project code no.	PB23				
Substance name	Urea, N-(4-chlorophenyl)-N'-(3,4-dichlorophenyl)-				
Synonyms					
CAS No	101-20-2		EINECS No	202-924-1	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP, US HPV
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	4.9 5.8–6	K_{ow} data type	Predicted Measured	Log K_{ow} source	EPI SUITE US HPV
BCF	137 81	BCF data type	Measured Measured	BCF source	US HPV CHRIP
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.00006				US HPV
Ecotoxicity comments					
Water solubility (mg/l)	0.0009			WS source	EPI SUITE
P classification	P (provisional)				
B classification	Not B (based on measured result accepted by regulatory authority)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Not PBT. T originally based on Danish EPA mutagenicity prediction				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	Web has use as anti-microbial agent (triclocarban) in personal care products.				
Potential for exposure over wide scale?	Yes, based on confidential use information and on web information				
Overall comments	High priority for further investigation				

Project code no.	PB25				
Substance name	Profenofos				
Synonyms					
CAS No	41198-08-7		EINECS No	255-255-2	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.82 4.68	K_{ow} data type	Predicted Measured	Log K_{ow} source	EPI SUITE CHRIP
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.101				ECOSAR
Ecotoxicity comments	T from N-Class entry (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	20			WS source	CHRIP
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)					
Summary of use	Web has use as insecticide				
Potential for exposure over wide scale?	Yes, based on confidential use information and on web information				
Overall comments	High priority for further investigation				

Project code no.	PB26				
Substance name	1,4-Pentanediamine, N(4)-(7-chloro-4-quinolinyl)-N(1),N(1)-diethyl-, phosphate (1:2)				
Synonyms					
CAS No	50-63-5		EINECS No	200-055-2	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.5	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.225			Ecotox source	ECOSAR
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity				
Water solubility (mg/l)	10.6			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	*Kirk-Othmer* has use as an antiprotozoal agent, OSPAR as a drug				
Potential for exposure over wide scale?	Yes, based on *Kirk-Othmer* and OSPAR use information				
Overall comments	High priority for further investigation				

Project code no.	PB27				
Substance name	Benzene, 1,2,4-trichloro-5-[(4-chlorophenyl)sulfonyl]-				
Synonyms					
CAS No	116-29-0	EINECS No		204-134-2	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.61	K_{ow} data type	Measured	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.058				ECOSAR
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.66			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has use as pesticide and acaricide; OSPAR has use as pesticide				
Potential for exposure over wide scale?	Yes, based on confidential use information and on *Kirk-Othmer*/OSPAR information				
Overall comments	High priority for further investigation				

Project code no.	PB28				
Substance name	Propanoic acid, 2-[4-(2,2-dichlorocyclopropyl)phenoxy]-2-methyl-, ethyl ester				
Synonyms					
CAS No	52179-28-9		EINECS No	257-709-5	
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.72	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.103				ECOSAR
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.9			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	No, as no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PB29				
Substance name	Benzenesulfonic acid, 2-amino-, (1-methylethylidene)di-4,1-phenylene ester				
Synonyms					
CAS No	68015-60-1	EINECS No	268-141-2		
Existing regulatory and related activity (e.g. priority lists)	OSPAR				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.63	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.021				ECOSAR
Ecotoxicity comments	T based on OSPAR identification as very toxic for ecotoxicity (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.04			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PB30				
Substance name	2,7-Naphthalenedisulfonic acid, 4-amino-3-[[4'-[(2,4-diaminophenyl)azo][1,1'-biphenyl]-4-yl]azo]-5-hydroxy-6-(phenylazo)-, disodium salt				
Synonyms					
CAS No	1937-37-7	EINECS No		217-710-3	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	CHRIP
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	4.9	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.445				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.00002			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)	Yes, on web				
Summary of use	Web has use as dye				
Potential for exposure over wide scale?	Yes, based on confidential use information and on web information				
Overall comments	High priority for further investigation				

Project code no.	PB31				
Substance name	Benzene, 1,3-bis(1-isocyanato-1-methylethyl)-				
Synonyms					
CAS No	2778-42-9	EINECS No	220-474-4		
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)	'Persistent' based on ready biodegradability test			Biodegradation source	US HPV
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments	Measured and predicted results in agreement				
Log K_{ow}	4.74	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.67			Ecotox source	US HPV
Lowest chronic ecotox NOEC (mg/l)	0.34				US HPV
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT (measured values would not indicate T)				
Water solubility (mg/l)	2.29			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)					
Summary of use	*Kirk-Othmer* has use as cross-linking agent for hydroxy-functional resins				
Potential for exposure over wide scale?	No, based on confidential use information and on *Kirk-Othmer* information				
Overall comments	Medium priority for further investigation				

Project code no.	PB32				
Substance name	2,4,11,13-Tetraazatetradecanediimidamide, N,N''-bis(4-chlorophenyl)-3,12-diimino-, diacetate				
Synonyms					
CAS No	56-95-1	EINECS No		200-302-4	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.85	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.484				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.05			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information				
Overall comments	High priority for further investigation				

Project code no.	PB33				
Substance name	1-Propanaminium, 3-[[9,10-dihydro-4-[(4-methylphenyl)amino]-9,10-dioxo-1-anthracenyl]amino]-N,N,N-trimethyl-, methyl sulfate				
Synonyms					
CAS No	72828-93-4		EINECS No	276-896-4	
Existing regulatory and related activity (e.g. priority lists)	Canadian DSL				
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.83	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.178				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT (ECOSAR prediction would not indicate T)				
Water solubility (mg/l)	0.002			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)					
Summary of use					
Potential for exposure over wide scale?	Yes, based on confidential use information but no current suppliers located				
Overall comments	Medium priority for further investigation				

Project code no.	PB34				
Substance name	Benzenesulfonamide, N-(4-amino-9,10-dihydro-3-methoxy-9,10-dioxo-1-anthracenyl)-4-methyl-				
Synonyms					
CAS No	81-68-5	EINECS No		201-369-2	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)				Biodegradation source	
Biodegradation (predicted)	Not readily biodegradable (REACH screening)			Biodegradation source	EPI SUITE
Biodegradation comments					
Log K_{ow}	4.79	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)				Ecotox source	
Lowest chronic ecotox NOEC (mg/l)	0.006				ECOSAR
Ecotoxicity comments	T based on Canadian DSL categorisation as PBiT				
Water solubility (mg/l)	0.01			WS source	EPI SUITE
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	T (provisional)	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Possible PBT				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	Web has use as dye				
Potential for exposure over wide scale?	Yes, based on confidential use information and on web information				
Overall comments	High priority for further investigation				

Project code no.	PB35				
Substance name	Ionone, methyl-				
Synonyms					
CAS No	1335-46-2	EINECS No		215-635-0	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)	Readily biodegradable (measured)			Biodegradation source	US HPV
Biodegradation (predicted)	Not readily biodegradable (report screening)			Biodegradation source	EA (in prep.)
Biodegradation comments	Measured result accepted by regulatory authority)				
Log K_{ow}	4.84	K_{ow} data type	Predicted	Log K_{ow} source	EPI SUITE
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	2.65			Ecotox source	US HPV
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments	Other similar values to measured result in CHRIP				
Water solubility (mg/l)	90			WS source	US HPV
P classification	Not P (based on measured result accepted by regulatory authority)				
B classification	B (provisional)				
T classification – aquatic only	Not T	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Not PBT (based on measured results accepted by regulatory authority)				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	EA (in prep.) has use in fragrances				
Potential for exposure over wide scale?	Yes, based on EA (in prep.)				
Overall comments	Low priority for further investigation				

Project code no.	PB36				
Substance name	3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one				
Synonyms					
CAS No	127-51-5	EINECS No		204-846-3	
Existing regulatory and related activity (e.g. priority lists)					
Biodegradation (measured)	Inherently biodegradable			Biodegradation source	US HPV
Biodegradation (predicted)	Not readily biodegradable (report screening)			Biodegradation source	EA (in prep.)
Biodegradation comments					
Log K_{ow}	4.84	K_{ow} data type	Predicted	Log K_{ow} source	EA (in prep.)
BCF		BCF data type		BCF source	
Lowest acute ecotox L(E)C50 (mg/l)	0.43			Ecotox source	EA (in prep.)
Lowest chronic ecotox NOEC (mg/l)					
Ecotoxicity comments					
Water solubility (mg/l)	16			WS source	US HPV
P classification	P (provisional)				
B classification	B (provisional)				
T classification – aquatic only	Not T	T classification overall (i.e. including mammalian toxicity)			
Comments on PBT screen	Not PBT				
Possible UK suppliers (with source)	Yes, in IUCLID 4				
Summary of use	EA (in prep.) has use in fragrances				
Potential for exposure over wide scale?	Yes, based on EA (in prep.)				
Overall comments	Low priority for further investigation				

Appendix 3 Substance lists

This appendix contains the complete lists of substances identified as PvB and PB through the processes in Section 2. It also presents the list of substances removed from consideration at the start of Section 3 as being already the subject of assessments in other fora.

Table A3.1 Initial list of potential PvB substances.

Code number	Source	CAS	Substance
PvB1	D(a)	10192-93-5	benzene, 1,1′-(1,2-diethyl-1,2-dimethyl-1,2-ethanediyl)bis-
PvB2	D(a)	104-42-7	benzenamine, 4-dodecyl-
PvB3	D(a)	11028-42-5	cedrene
PvB4	D(a)	112-29-8	decane, 1-bromo-
PvB5	D(a)	120-95-6	phenol, 2,4-bis(1,1-dimethylpropyl)-
PvB6	D(a)	128-69-8	perylo[3,4-cd:9,10-c′d′]dipyran-1,3,8,10-tetrone
PvB7	D(a)	129-73-7	benzenamine, 4,4′-(phenylmethylene)bis[N,N-dimethyl-
PvB8	D(a)	13393-93-6	1-phenanthrenemethanol, tetradecahydro-1,4a-dimethyl-7-(1-methylethyl)-
PvB9	D(a)	135-91-1	benzenamine, 4,4′-methylenebis[N,N-diethyl-
PvB10	D(a)	13680-35-8	benzenamine, 4,4′-methylenebis[2,6-diethyl-
PvB11	D(a)	139-60-6	1,4-benzenediamine, N,N′-bis(1-ethyl-3-methylpentyl)-
PvB12	D(a)	1484-08-8	9H-carbazole, 9-butyl-
PvB13	D(a)	15233-47-3	1,4-benzenediamine, N-(1-methylheptyl)-N′-phenyl-
PvB14	D(a)	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)-
PvB15	D(a)	17540-75-9	phenol, 2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-
PvB16	D(a)	18254-13-2	phenol, 2,4,6-tris(1-phenylethyl)-
PvB17	D(a)	1889-67-4	benzene, 1,1′-(1,1,2,2-tetramethyl-1,2-ethanediyl)bis-
PvB18	D(a)	19941-28-7	1-phenanthrenecarboxylic acid, tetradecahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1alpha,4abeta,4balpha,7beta,8abeta,10aalpha)]-
PvB19	D(a)	23593-75-1	1H-imidazole, 1-[(2-chlorophenyl)diphenylmethyl]-
PvB20	D(a)	2422-91-5	benzene, 1,1′,1″-methylidynetris[4-isocyanato-
PvB21	D(a)	25973-55-1	phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)-
PvB22	D(a)	29312-59-2	benzenamine, 4-(2,6-diphenyl-4-pyridinyl)-N,N-dimethyl-
PvB23	D(a)	29398-96-7	[1,1′-biphenyl]-4,4′-diamine, N,N′-bis(2,4-dinitrophenyl)-3,3′-dimethoxy-
PvB24	D(a)	3081-01-4	1,4-benzenediamine, N-(1,4-dimethylpentyl)-N′-phenyl-
PvB25	D(a)	3147-75-9	phenol, 2-(2H-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)-
PvB26	D(a)	32388-55-9	ethanone, 1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)-, [3R-(3alpha,3abeta,7beta,8aalpha)]-
PvB27	D(a)	3271-22-5	1,3,5-triazine, 2,4-dimethoxy-6-(1-pyrenyl)-
PvB28	D(a)	3278-89-5	benzene, 1,3,5-tribromo-2-(2-propenyloxy)-
PvB29	D(a)	335-57-9	heptane, hexadecafluoro-
PvB30	D(a)	3407-42-9	cyclohexanol, 3-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)-
PvB31	D(a)	355-42-0	hexane, tetradecafluoro-
PvB32	D(a)	355-43-1	hexane, 1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-6-iodo-

Code number	Source	CAS	Substance
PvB33	D(a)	36437-37-3	phenol, 2-(2H-benzotriazol-2-yl)-4-(1,1-dimethylethyl)-6-(1-methylpropyl)-
PvB34	D(a)	3739-67-1	benzene, 1,1′-(1-methylethylidene)bis[4-(2-propenyloxy)-
PvB35	D(a)	3846-71-7	phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)-
PvB36	D(a)	38521-51-6	benzene, pentabromo(bromomethyl)-
PvB37	D(a)	3864-99-1	phenol, 2-(5-chloro-2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)-
PvB38	D(a)	40567-16-6	butanoyl chloride, 2-[2,4-bis(1,1-dimethylpropyl)phenoxy]-
PvB39	D(a)	4130-42-1	phenol, 2,6-bis(1,1-dimethylethyl)-4-ethyl-
PvB40	D(a)	4162-45-2	ethanol, 2,2′-[(1-methylethylidene)bis[(2,6-dibromo-4,1-phenylene)oxy]]bis-
PvB41	D(a)	42074-68-0	benzene, 1-chloro-2-(chlorodiphenylmethyl)-
PvB42	D(a)	423-50-7	1-hexanesulfonyl fluoride, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-
PvB43	D(a)	4378-61-4	dibenzo[def,mno]chrysene-6,12-dione, 4,10-dibromo-
PvB44	D(a)	469-61-4	1H-3a,7-methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3alpha,3abeta,7beta,8aalpha)]-
PvB45	D(a)	50772-29-7	butanoyl chloride, 4-[2,4-bis(1,1-dimethylpropyl)phenoxy]-
PvB46	D(a)	512-04-9	spirost-5-en-3-ol, (3beta,25R)-
PvB47	D(a)	51630-58-1	benzeneacetic acid, 4-chloro-alpha-(1-methylethyl)-, cyano(3-phenoxyphenyl)methyl ester
PvB48	D(a)	5165-81-1	2-naphthalenecarboxamide, N-(4-chloro-2-methoxy-5-methylphenyl)-3-hydroxy-
PvB49	D(a)	52434-90-9	1,3,5-triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris(2,3-dibromopropyl)-
PvB50	D(a)	52740-90-6	2-anthracenecarboxamide, 1-amino-N-(3-bromo-9,10-dihydro-9,10-dioxo-2-anthracenyl)-9,10-dihydro-9,10-dioxo-
PvB51	D(a)	5285-60-9	benzenamine, 4,4′-methylenebis[N-(1-methylpropyl)-
PvB52	D(a)	54079-53-7	propanedinitrile, [[4-[[2-(4-cyclohexylphenoxy)ethyl]ethylamino]-2-methylphenyl]methylene]-
PvB53	D(a)	54914-37-3	cyclohexanemethanamine, 1,3,3-trimethyl-N-(2-methylpropylidene)-5-[(2-methylpropylidene)amino]-
PvB54	D(a)	55525-54-7	urea, N,N′-bis[(5-isocyanato-1,3,3-trimethylcyclohexyl)methyl]-
PvB55	D(a)	56358-17-9	2-naphthalenamine, N-(2-ethylhexyl)-
PvB56	D(a)	59447-55-1	2-propenoic acid, (pentabromophenyl)methyl ester
PvB57	D(a)	63059-55-2	hexanoyl chloride, 2-[2,4-bis(1,1-dimethylpropyl)phenoxy]-
PvB58	D(a)	63216-89-7	1H-indene-1,3(2H)-dione, 2-benzo[f]quinolin-3-yl-
PvB59	D(a)	732-26-3	phenol, 2,4,6-tris(1,1-dimethylethyl)-
PvB60	D(a)	79-74-3	1,4-benzenediol, 2,5-bis(1,1-dimethylpropyl)-
PvB61	D(a)	850-92-0	1,3-cyclopentanedione, 2-[2-(3,4-dihydro-6-methoxy-1(2H)-naphthalenylidene)ethyl]-2-ethyl-
PvB62	D(a)	85-22-3	benzene, pentabromoethyl-
PvB63	D(a)	87-83-2	benzene, pentabromomethyl-
PvB64	D(a)	90-93-7	methanone, bis[4-(diethylamino)phenyl]-
PvB65	D(a)	93-46-9	1,4-benzenediamine, N,N′-di-2-naphthalenyl-
PvB66	D(b)	128-70-1	8,16-pyranthrenedione
PvB67	D(b)	135-65-9	2-naphthalenecarboxamide, 3-hydroxy-N-(3-nitrophenyl)-

Code number	Source	CAS	Substance
PvB68	N	13121-70-5	stannane, tricyclohexylhydroxy-
PvB69	N	13356-08-6	distannoxane, hexakis(2-methyl-2-phenylpropyl)-
PvB70	N	15696-43-2	octanoic acid, lead salt
PvB71	N	2223-93-0	octadecanoic acid, cadmium salt
PvB72	N	309-00-2	1,4:5,8-dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1.alpha.,4.alpha.,4a.beta.,5.alpha.,8.alpha.,8a.beta.)-
PvB73	N	3091-32-5	stannane, chlorotricyclohexyl-
PvB74	N	32534-81-9	benzene, 1,1′-oxybis-, pentabromo derivative
PvB75	N	3861-47-0	octanoic acid, 4-cyano-2,6-diiodophenyl ester
PvB76	N	40487-42-1	benzenamine, N-(1-ethylpropyl)-3,4-dimethyl-2,6-dinitro-
PvB77	N	41083-11-8	1H-1,2,4-triazole, 1-(tricyclohexylstannyl)-
PvB78	N	52315-07-8	cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester (cypermethrin)
PvB79	N	52645-53-1	cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, (3-phenoxyphenyl)methyl ester
PvB80	N	61951-96-0	neodecanoic acid, cadmium salt
PvB81	N	67375-30-8	cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester (alpha-cypermethrin)
PvB82	O	81-98-1	7H-benz[de]anthracen-7-one, 3,9-dibromo-
PvB83	O	128-83-6	perylo[3,4-cd:9,10-c′d′]dipyran-1,3,8,10-tetrone
PvB84	O	375-72-4	1-butanesulfonyl fluoride, 1,1,2,2,3,3,4,4,4-nonafluoro-
PvB85	O	632-79-1	1,3-isobenzofurandione, 4,5,6,7-tetrabromo-
PvB86	O	1861-40-1	benzenamine, N-butyl-N-ethyl-2,6-dinitro-4-(trifluoromethyl)-
PvB87	O	4051-63-2	[1,1′-bianthracene]-9,9′,10,10′-tetrone, 4,4′-diamino-
PvB88	O	7139-02-8	pyrimido[5,4-d]pyrimidine, 2,6-dichloro-4,8-di-1-piperidinyl-
PvB89	O	15114-15-5	9,10-anthracenedione, 4,8-diamino-2-(4-ethoxyphenyl)-1,5-dihydroxy-
PvB90	O	19774-82-4	methanone, (2-butyl-3-benzofuranyl)[4-[2-(diethylamino)ethoxy]-3,5-diiodophenyl]-, hydrochloride
PvB91	O	21850-44-2	benzene, 1,1′-(1-methylethylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)-
PvB92	O	36861-47-9	bicyclo(2.2.1)heptan-2-one, 1,7,7-trimethyl-3-[(4-methylphenyl)methylene]-
PvB93	O	38521-51-6	benzene, pentabromo(bromomethyl)-
PvB94	O	39489-75-3	phenol, 2,4-dichloro-5-nitro-, carbonate (2:1) (ester)
PvB95	O	41999-84-2	benzene, 1,4-dichloro-2,5-bis(dichloromethyl)-
PvB96	O	68085-85-8	cyclopropanecarboxylic acid, 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethyl-, cyano(3-phenoxyphenyl)methyl ester
PvB97	DSL-E	1068-27-5	peroxide, (1,1,4,4-tetramethyl-2-butyne-1,4-diyl)bis[(1,1-dimethylethyl)
PvB98	DSL-E	12236-64-5	2-naphthalenecarboxamide, N-[4-(acetylamino)phenyl]-4-[[5-(aminocarbonyl)-2-chlorophenyl]azo]-3-hydroxy-
PvB99	DSL-E	12239-34-8	acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-ethoxyphenyl]-
PvB100	DSL-E	1229-55-6	2-naphthalenol, 1-[(2-methoxyphenyl)azo]-
PvB101	DSL-E	14295-43-3	benzo[b]thiophen-3(2H)-one, 4,7-dichloro-2-(4,7-dichloro-3-oxobenzo[b]thien-2(3H)-ylidene)-
PvB102	DSL-E	15086-94-9	spiro[isobenzofuran-1(3H),9′-[9H]xanthen]-3-one, 2′,4′,5′,7′-tetrabromo-3′,6′-dihydroxy-

Code number	Source	CAS	Substance
PvB103	DSL-E	15958-61-9	9,10-anthracenedione, 1-[[4-(phenylsulfonyl)phenyl]amino]-
PvB104	DSL-E	17464-91-4	ethanol, 2,2′-[[4-[(2-bromo-6-chloro-4-nitrophenyl)azo]-3-chlorophenyl]imino]bis-
PvB105	DSL-E	19800-42-1	phenol, 4-[[2-methoxy-4-[(4-nitrophenyl)azo]phenyl]azo]-
PvB106	DSL-E	20241-76-3	9,10-anthracenedione, 1,8-dihydroxy-4-nitro-5-(phenylamino)-
PvB107	DSL-E	23355-64-8	ethanol, 2,2′-[[3-chloro-4-[(2,6-dichloro-4-nitrophenyl)azo]phenyl]imino]bis-
PvB108	DSL-E	2425-85-6	2-naphthalenol, 1-[(4-methyl-2-nitrophenyl)azo]-
PvB109	DSL-E	24610-00-2	benzonitrile, 2-[[4-[(2-cyanoethyl)(2-phenylethyl)amino]phenyl]azo]-5-nitro-
PvB110	DSL-E	25155-25-3	peroxide, [1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[(1,1-dimethylethyl)
PvB111	DSL-E	2814-77-9	2-naphthalenol, 1-[(2-chloro-4-nitrophenyl)azo]-
PvB112	DSL-E	3468-63-1	2-naphthalenol, 1-[(2,4-dinitrophenyl)azo]-
PvB113	DSL-E	42739-61-7	nickel, bis[2,3-bis(hydroxyimino)-N-(2-methoxyphenyl)butanamidato]-
PvB114	DSL-E	43035-18-3	benzenesulfonic acid, 4-[[3-[[2-hydroxy-3-[[(4-methoxyphenyl)amino]carbonyl]-1-naphthalenyl]azo]-4-methylbenzoyl]amino]-, calcium salt (2:1)
PvB115	DSL-E	475-71-8	benzo[h]benz[5,6]acridino[2,1,9,8-klmna]acridine-8,16-dione
PvB116	DSL-E	509-34-2	spiro[isobenzofuran-1(3H),9′-[9H]xanthen]-3-one, 3′,6′-bis(diethylamino)-
PvB117	DSL-E	5261-31-4	propanenitrile, 3-[[2-(acetyloxy)ethyl][4-[(2,6-dichloro-4-nitrophenyl)azo]phenyl]amino]-
PvB118	DSL-E	52697-38-8	acetamide, N-[2-[(2-bromo-4,6-dinitrophenyl)azo]-5-(diethylamino)phenyl]-
PvB119	DSL-E	53184-75-1	phosphorous acid, (1-methylethylidene)di-4,1-phenylene tetrakis[(3-ethyl-3-oxetanyl)methyl] ester
PvB120	DSL-E	540-97-6	cyclohexasiloxane, dodecamethyl-
PvB121	DSL-E	59487-23-9	2-naphthalenecarboxamide, 4-[[5-[[[4-(aminocarbonyl) phenyl]amino]carbonyl]-2-methoxyphenyl]azo]-N-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxy-
PvB122	DSL-E	59709-10-3	pyridinium, 1-[2-[[4-[(2-chloro-4-nitrophenyl)azo]phenyl]ethylamino]ethyl]-, acetate
PvB123	DSL-E	59709-38-5	β-alanine, N-[4-[(2-bromo-6-chloro-4-nitrophenyl)azo]phenyl]-N-(3-methoxy-3-oxopropyl)-, methyl ester
PvB124	DSL-E	6250-23-3	phenol, 4-[[4-(phenylazo)phenyl]azo]-
PvB125	DSL-E	6407-78-9	3H-pyrazol-3-one, 4-[(2,4-dimethylphenyl)azo]-2,4-dihydro-5-methyl-2-phenyl-
PvB126	DSL-E	6410-41-9	2-naphthalenecarboxamide, N-(5-chloro-2,4-dimethoxyphenyl)-4-[[5-[(diethylamino)sulfonyl]-2-methoxyphenyl]azo]-3-hydroxy-
PvB127	DSL-E	64338-16-5	7-oxa-3,20-diazadispiro[5.1.11.2]heneicosan-21-one, 2,2,4,4-tetramethyl-
PvB128	DSL-E	65140-91-2	phosphonic acid, [[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-, monoethyl ester, calcium salt (2:1)
PvB129	DSL-E	6731-36-8	peroxide, (3,3,5-trimethylcyclohexylidene)bis[(1,1-dimethylethyl)
PvB130	DSL-E	6786-83-0	1-naphthalenemethanol, α,α-bis[4-(dimethylamino) phenyl]-4-(phenylamino)-
PvB131	DSL-E	68391-08-2	alcohols, C8–14, γ-ω-perfluoro
PvB132	DSL-E	68877-63-4	acetamide, N-[2-[(2-bromo-4,6-dinitrophenyl)azo]-5-[(2-cyanoethyl)-2-propenylamino]-4-methoxyphenyl]-
PvB133	DSL-E	70331-94-1	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, (1,2-dioxo-1,2-ethanediyl)bis(imino-2,1-ethanediyl) ester
PvB134	DSL-E	70660-55-8	1-naphthalenamine, 4-[(2-bromo-4,6-dinitrophenyl)azo]-N-(3-methoxypropyl)-
PvB135	DSL-E	72869-85-3	chromate(1-), bis[3,5-bis(1,1-dimethylethyl)-2-hydroxybenzoato(2-)-O1,O2]-, hydrogen
PvB136	DSL-E	72968-82-2	methanesulfonamide, N-[2-[(2,6-dicyano-4-methylphenyl)azo]-5-(dipropylamino)phenyl]-
PvB137	DSL-E	74336-60-0	9,10-anthracenedione, 1-[(5,7-dichloro-1,9-dihydro-2-methyl-9-oxopyrazolo[5,1-b]quinazolin-3-yl)azo]-

Code number	Source	CAS	Substance
PvB138	DSL-E	78-63-7	peroxide, (1,1,4,4-tetramethyl-1,4-butanediyl)bis[(1,1-dimethylethyl)
PvB139	DSL-E	83006-67-1	benzenesulfonic acid, 2,2′-[(9,10-dihydro-5,8-dihydroxy-9,10-dioxo-1,4-anthracenediyl)diimino]bis[5-(1,1-dimethylethyl)-, disodium salt
PvB140	DSL-E	85702-64-3	3H-indol-3-one, 5,7-dibromo-2-(5-bromo-7-chloro-1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-
PvB141	DSL-E	85-86-9	2-naphthalenol, 1-[[4-(phenylazo)phenyl]azo]-
PvB142	DSL-H	842-07-9	2-naphthalenol, 1-(phenylazo)-
PvB143	HSE-R48	67-97-0	colecalciferol, Vitamin D3
PvB144	F	21145-77-7	1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthyl)ethan-1-one
PvB145	F	28219-61-6	2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol
PvB146	F	28371-99-5	methyl 2,6,10-trimethylcyclododeca-2,5,9-trien-1-yl ketone
PvB147	F	13171-00-1	6-tert-butyl-1,1-dimethylindan-4-yl methyl ketone
PvB148	F	87-44-5	Caryophyllene
PvB149	F	65113-99-7	a,b,2,2,3-pentamethylcyclopent-3-ene-1-butanol
PvB150	F	77-54-3	[3R-(3a,3ab,6a,7b,8aa)]-octahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl acetate
PvB151	FR	96-69-5	4,4′-thio-bis(2-t-butyl-5-methylphenol)
PvB152	FR	13560-89-9	dodecachlorodimethan-o-dibenzocyclooctane
PvB153	FR	25327-89-3	tetrabromobisphenol-A bis(allylether)
PvB154	FR	26040-51-7	phthalic acid, tetrabromo-, bis(2-ethylhexyl) ester
PvB155	FR	58965-66-5	tetradecabromodiphenoxybenzene
PvB156	UV	118-56-9	homosalate
PvB157	UV	21245-02-3	ethylhexyl dimethyl PABA
PvB158	UV	6197-30-4	Octocrylene
PvB159	UV	15087-24-8	3-benzylidene camphor

Source: D(a), Danish EPA database R50/53; D(b), Danish EPA database R51/53+Mut3; N, N-Class; O, OSPAR list; DSL-E, Canadian PBiT list; DSL-H, Canadian PBiThuman list; HSE-R48, HSE R48 list; F, the fragrance-sector report; FR, flame-retardants sector report; UV, UV-filters report. See Section 2.2 for more information.

Table A3.2 Initial list of potential PB substances.

Code number	Source	CAS	Substance
PB1	D(a)	10310-32-4	D-glucofuranoside, ethyl 3,5,6-tris-O-(phenylmethyl)-
PB2	D(a)	119-94-8	benzenemethanamine, N-ethyl-N-(3-methylphenyl)-
PB3	D(a)	129-00-0	Pyrene
PB4	D(a)	133-91-5	benzoic acid, 2-hydroxy-3,5-diiodo-
PB5	D(a)	15307-93-4	benzenamine, 2,6-dichloro-N-phenyl-

Code number	Source	CAS	Substance
PB6	D(a)	3380-34-5	phenol, 5-chloro-2-(2,4-dichlorophenoxy)-
PB7	D(a)	41604-19-7	1,1′-biphenyl, 4-bromo-2-fluoro-
PB8	D(a)	4273-92-1	2-naphthalenecarboxamide, N-(4-chloro-2,5-dimethoxyphenyl)-3-hydroxy-
PB9	D(a)	43076-61-5	1-butanone, 4-chloro-1-[4-(1,1-dimethylethyl)phenyl]-
PB10	D(a)	464-41-5	bicyclo[2.2.1]heptane, 2-chloro-1,7,7-trimethyl-, endo-
PB11	D(a)	467-63-0	benzenemethanol, 4-(dimethylamino)-alpha,alpha-bis[4-(dimethylamino)phenyl]-
PB12	D(a)	50-65-7	benzamide, 5-chloro-N-(2-chloro-4-nitrophenyl)-2-hydroxy-
PB13	D(a)	51-03-6	1,3-benzodioxole, 5-[[2-(2-butoxyethoxy)ethoxy]methyl]-6-propyl-
PB14	D(a)	57018-04-9	phosphorothioic acid, O-(2,6-dichloro-4-methylphenyl) O,O-dimethyl ester
PB15	D(a)	626-39-1	benzene, 1,3,5-tribromo-
PB16	D(a)	634-66-2	benzene, 1,2,3,4-tetrachloro-
PB17	D(a)	63734-62-3	benzoic acid, 3-[2-chloro-4-(trifluoromethyl)phenoxy]-
PB18	D(a)	66063-05-6	urea, N-[(4-chlorophenyl)methyl]-N-cyclopentyl-N′-phenyl-
PB19	D(a)	7785-70-8	bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-, (1R)-
PB20	D(a)	82-05-3	7H-benz[de]anthracen-7-one
PB21	D(a)	87-68-3	1,3-butadiene, 1,1,2,3,4,4-hexachloro-
PB22	D(a)	92-72-8	2-naphthalenecarboxamide, N-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxy-
PB23	D(b)	101-20-2	urea, N-(4-chlorophenyl)-N′-(3,4-dichlorophenyl)-
PB24	N	117-08-8	1,3-isobenzofurandione, 4,5,6,7-tetrachloro-
PB25	N	41198-08-7	Profenofos
PB26	O	50-63-5	1,4-pentanediamine, N(4)-(7-chloro-4-quinolinyl)-N(1),N(1)-diethyl-, phosphate (1:2)
PB27	O	116-29-0	benzene, 1,2,4-trichloro-5-[(4-chlorophenyl)sulfonyl]-
PB28	O	52179-28-9	propanoic acid, 2-[4-(2,2-dichlorocyclopropyl)phenoxy]-2-methyl-, ethyl ester
PB29	O	68015-60-1	benzenesulfonic acid, 2-amino-, (1-methylethylidene)di-4,1-phenylene ester
PB30	DSL-E	1937-37-7	2,7-naphthalenedisulfonic acid, 4-amino-3-[[4′-[(2,4-diaminophenyl)azo][1,1′-biphenyl]-4-yl]azo]-5-hydroxy-6-(phenylazo)-, disodium salt
PB31	DSL-E	2778-42-9	benzene, 1,3-bis(1-isocyanato-1-methylethyl)-
PB32	DSL-E	56-95-1	2,4,11,13-tetraazatetradecanediimidamide, N,N″-bis(4-chlorophenyl)-3,12-diimino-, diacetate
PB33	DSL-E	72828-93-4	1-propanaminium, 3-[[9,10-dihydro-4-[(4-methylphenyl)amino]-9,10-dioxo-1-anthracenyl]amino]-N,N,N-trimethyl-, methyl sulfate
PB34	DSL-E	81-68-5	benzenesulfonamide, N-(4-amino-9,10-dihydro-3-methoxy-9,10-dioxo-1-anthracenyl)-4-methyl-
PB35	F	1335-46-2	ionone, methyl -
PB36	F	127-51-5	3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one

Source: D(a), Danish EPA database R50/53; D(b), Danish EPA database R51/53+Mut3; N, N-Class; O, OSPAR list; DSL-E, Canadian PBiT list; F, fragrance-sector report. See Section 2.2 for more information.

Table A3.3 Substances removed from list as already assessed elsewhere.

Code number	Source	CAS	Substance	Reason for removal
PvB5	D(a)	120-95-6	phenol, 2,4-bis(1,1-dimethylpropyl)-	EA complex cresols and phenols assessment
PvB6	D(a)	128-69-8	perylo[3,4-cd:9,10-c′d′]dipyran-1,3,8,10-tetrone	EU PBT WG – deselected (not B)
PvB14	D(a)	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)-	PFOS assessment
PvB16	D(a)	18254-13-2	phenol, 2,4,6-tris(1-phenylethyl-)	Styrenated phenol CCRMP assessment (tri-stryenated component)
PvB44	D(a)	469-61-4	1H-3a,7-methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3alpha,3abeta,7beta,8aalpha)]-	EU PBT WG – deselected (not P)
PvB60	D(a)	79-74-3	1,4-benzenediol, 2,5-bis(1,1-dimethylpropyl)-	EA complex cresols and phenols assessment
PvB74	N	32534-81-9	benzene, 1,1′-oxybis-, pentabromo derivative [pentabromodiphenyl ether]	ESR assessment
PvB94	O	39489-75-3	phenol, 2,4-dichloro-5-nitro-, carbonate (2:1) (ester)	EU PBT WG – deferred (reason unclear)
PvB120	DSL-E	540-97-6	cyclohexasiloxane, dodecamethyl-	Siloxanes CCRMP assessment (D6)
PB21	D(a)	87-68-3	1,3-butadiene, 1,1,2,3,4,4-hexachloro-	EU PBT WG
PB24	N	117-08-8	1,3-isobenzofurandione, 4,5,6,7-tetrachloro- [Tetrachlorophthalic anhydride]	EU PBT WG – deselected (not P due to fast hydrolysis)

Source: D(a), Danish EPA database R50/53; N, N-Class; O, OSPAR list; DSL-E, Canadian PBiT list. See Section 2.2 for more information.

Appendix 4 Unreviewed substances

This appendix lists the LPV substances identified as candidate substances from the source lists in Section 2.2, but for which there was no match in the CAS number database in EPI SUITE. They could be re-examined if REACH registrations are made in future.

Danish EPA

CAS	Substance
1779-51-7	phosphonium, butyltriphenyl-, bromide
2751-90-8	phosphonium, tetraphenyl-, bromide
456-04-2	ethanone, 2-chloro-1-(4-fluorophenyl)-
4682-36-4	ethanamine, N,N-dimethyl-2-[(2-methylphenyl)phenylmethoxy]-, 2-hydroxy-1,2,3-propanetricarboxylate (1:1)
64131-85-7	phosphorothioic acid, O,O,O-tris(4-nitrophenyl) ester

OSPAR

CAS	Substance
9016-45-9	nonylphenol ethoxylate[29]
65294-17-9	methylium, tris[4-(dimethylamino)phenyl]-, salt with 3-[[4-(phenylamino)phenyl]azo]-benzenesulfonic acid (1:1)
70776-03-3	naphthalene, chloro derivatives
90481-05-3	phenol, nonyl-, manufacture of, by-products from, high-boiling[30]

N-Class

CAS	Substance
10196-67-5	tetradecanoic acid, cadmium salt
10468-30-1	9-octadecenoic acid (Z)-, cadmium salt
2605-44-9	dodecanoic acid, cadmium salt
26354-18-7	2-propenoic acid, 2-methyl-, methyl ester, polymer with tributyl[(2-methyl-1-oxo-2-propenyl)oxy]stannane
53404-61-8	propanoic acid, 2-(4-chloro-2-methylphenoxy)-, compared with 2,2′,2″-nitrilotris[ethanol] (1:1)
61790-14-5	naphthenic acid, lead salt
68131-73-7	amines, polyethylenepoly-
68603-83-8	fatty acids, C6–19-branched, basic lead and lead salts
68953-39-9	fatty acids, tallow, hydroxylated, cadmium salts
83918-57-4	1H-imidazole, 1-[2-(2,4-dichlorophenyl)-2-(2-propenyloxy)ethyl]-, (.+-.)-, sulfate (1:1)
85409-17-2	stannane, tributyl-, mono(naphthenoyloxy) derivatives
90193-83-2	1,2-benzenedicarboxylic acid, lead(2+) salt, basic
90268-59-0	2-butenedioic acid (E)-, lead(2+) salt, basic
90431-26-8	isooctanoic acid, lead salt, basic
90431-40-6	lead, isononanoate naphthenate complexes, basic
90431-42-8	lead, isooctanoate naphthenate complexes, basic
91031-62-8	fatty acids, C16–18, lead salts
91078-81-8	naphthenic acids, lead (2+) salts
93981-67-0	isooctanoic acid, lead(2+) salt

[29] This substance is currently being assessed by the Environment Agency as part of a report on nonylphenol. It is not considered to be persistent.

[30] This product is mainly composed of dinonylphenol, and has been considered by the EU PBT WG (see Section 4.3) and addressed in an unpublished Environment Aagency risk evaluation report.

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