18 November 2013

Substance Brief Profiles Workshop

Background information

This paper is a "document in progress" reflecting the current status of ECHA proposal for Substance Brief Profiles.

Contents

1. Introduction

Dissemination is one of the pillars of REACH aiming at increasing the knowledge of the public about the properties of the chemical substances to which they may be exposed. It plays a pivotal role in assuring the safe use of chemicals, in terms of human health and environment, by placing information under the scrutiny of industry, downstream users and the general public.

ECHA is already publishing on its website a significant amount of information on chemicals. such as information on more than 11 000 substances from over 41 500 registration dossiers, EU harmonised classification for approximately 4 500 substances and Classification for more than 110 000 substances. In addition, information and lists of the various regulatory processes such as Candidate List, REACH Annex XIV ("Authorisation List") and Annex XVII ("Restriction List"), CoRAP for substance evaluation, Registry of intentions, Evaluation decisions, etc. are constantly being populated and published in various sections of the ECHA website.

REACH's goal is to increase the knowledge of the public about the properties of chemical substances.

In 2012 ECHA launched a Stakeholder Engagement Study aimed at better perceiving the requirements and needs of ECHA stakeholders when accessing ECHA's website. One of the main outcomes of the study was the need for user-friendly access to summarised information (or factsheets) and to download functionalities.

The access to summarised information is covered by recital 117 that defines that *"EU citizens should have access to information about chemicals to which they may be exposed, in order to allow them to make informed decisions about their use of chemicals. A transparent means of achieving this is to grant them free and easy access to basic data held in the Agency's database, including brief profiles of hazardous properties, labelling requirements and relevant Community legislation including authorised uses and risk management measures (…)".*

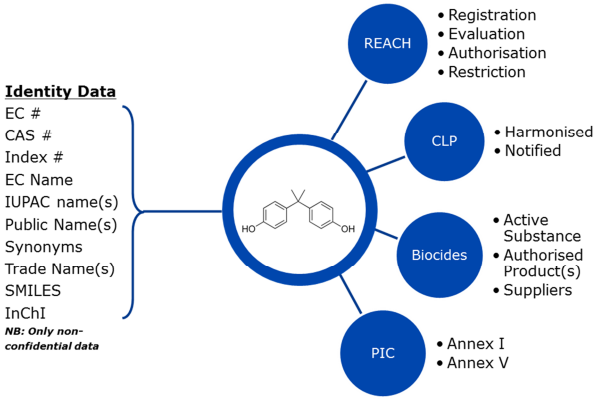
Giving stakeholders requirements and legal obligations, it is ECHA's ambition to improve the usability and user friendliness of the vast quantity of data on chemical substances that it has already published.

The following document provides information of ECHA's proposal for achieving these objectives.

2. Substance Centric Approach

In the current ECHA website data on substances is published separately by regulation and regulatory process. The first proposal to unify and better link data together is to move towards a substance centric approach:

Figure 1 – Substance centric model overview



With this approach each substance will have a single entry in a **Substance Master List**. This entry will contain all of the non-confidential identifying data for the substance, and will be linked to each regulation and regulatory process which touches on the substance.

3. Tiered Approach

As the information published by ECHA is vast and often very highly technical, a second proposal towards achieving the vision of improving the usability and user friendliness of the vast quantity of data published is to adopt a tiered approach. The aim is to present summarised tiers of information, as illustrated in the diagram below, with each tier tailored to different audiences with different levels of expertise:

Figure 2 – Tiered approach overview

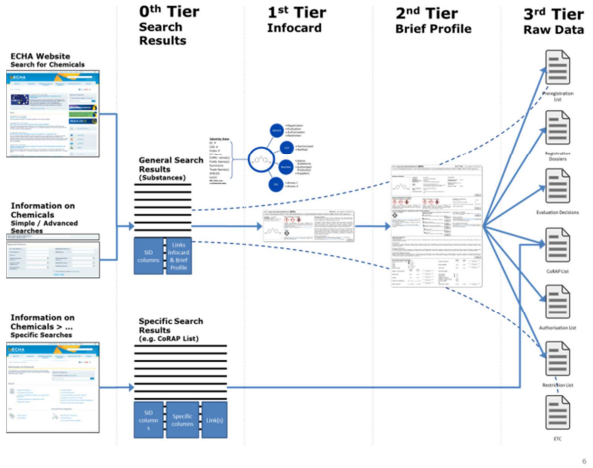


Table 3 – Tiered approach summary

Tiered approach to publishing information		
Tier	**Overview**	**Target Audience**
0	**Search results** – returned by substance search functions on the ECHA website. Row(s) of results containing columns – standard substance ID columns (e.g. EC, CAS, Substance Name) plus specific columns depending on the precise location on the ECHA website and the specific search function used.	General public
1	**Infocard** – a simple high-level summary of information on a substance. This would be designed to be understandable by the broadest possible audience and to contain the most relevant data (e.g. Classification and Labelling, Uses, main regulatory processes). Each row in the search results would be expandable into an Infocard.	Concerned citizens
2	**Brief Profile** – a summary of all the information held in ECHA's databases on a substance. This would contain an overview of every regulation and regulatory process or list that is relevant to the substance, and summarised scientific data on the substance.	Informed citizens
3	**Raw Data** – the full datasets of every regulation and regulatory list or process; what is currently published on the ECHA website.	Experts

4. Brief Profiles

A brief profile is proposed to be a useful and user friendly summary of all the data held in ECHA's databases relating to a substance. This would contain an overview of every regulation and regulatory process or list that is relevant to the substance, and summarised scientific data on the substance. A description of the data contained, and its derivation and display, is given below for each section of the brief profile proposed.

4.1. Header

The header of the brief profile will contain the ECHA Substance Name and the last updated date of the brief profile. It is also proposed to show synonyms in a second line, in alphabetical order, truncating those which do not fit and displaying only on mouse-over.

4.2. Introduction

This section will contain a very brief sentence about brief profiles, how they are generated and created, and reinforcing that they are generated automatically based on all the non-confidential information in EHCA's databases.

'More' links to an About Brief Profiles page on ECHA website giving more detailed background information.

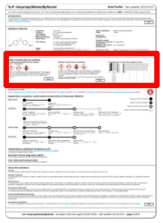
4.3. Substance Identity

This section will allow full identification of a substance and it is to be populated from data contained in the proposed ECHA **Substance Master List**. This section will contain the non-confidential substance identifying data, such as:

- Numerical identifiers – EC, CAS and Index numbers
- Key names for the substance – EC name, IUPAC name, CLP Annex VI Index names, synonyms
- Structural data – Smiles, InChI and a molecular structure image generated from these, molecular formula
- Type of substance and origin
- Composition, impurity and additive data
- Substance listed in: EINECS, ELINCS, NLP, REACH List number

'More' links to substance identity section(s) of registration dossier(s) for the substance.

4.4. Safety Classification and Labelling



This section is designed to provide a user friendly interpretation of the classification and labelling of the substance, as well as a full overview of all the classifications and labellings notified to ECHA for the substance. It will be divided in three sections:

- EU Harmonised Classification & Labelling – derived from the harmonised C&L(s) if extant. 'More' links to harmonised C&L entry in C&L Inventory.
- Notified Classifications & Labellings – derived from all notified classifications and labellings. 'More' links to notified C&L entries in C&L Inventory.
- Breakdown of notifications – graphical overview of all data in C&L inventory; harmonised and notified classifications, indicating agreement of joint entry and breakdown by % of notifications agreeing with a given H-code.

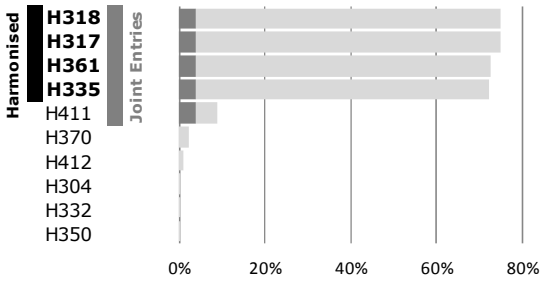
4.4.1. C&L Algorithm Logic Summary

1. Same logic applies to harmonised and notified data.
2. Count entries for pictograms; remove outlier(s); rank pictograms by number of entries; display in rank order. NB: No outliers will exist for harmonised data.
3. Count entries for hazard codes (H-codes); remove outlier(s); determine most severe H-code. NB: No outliers will exist for harmonised data.
4. Select framing text based on most severe H-Code (e.g. it is proposed EXTREME Caution, Caution, Take care, and Note, corresponding approximately to Fatal, Highly toxic, Toxic, and Harmful severities).
5. Rank H-codes by severity and by number of entries; display user friendly text per H-code in rank order.

4.4.2. C&L Graphical Breakdown

Graphical illustration of most notified H-codes (with mouse-over explanatory text). Illustrates harmonised codes, jointly entered codes, % of notifications with each code, % of joint and other notifications:

Figure 4 – Example C&L breakdown – Bisphenol-A



4.5. Concerns & Regulations / Regulatory Action on this substance

This section summarises the key concerns for a substance and the regulations which affect the substance.

4.5.1. Summary of concerns

Here certain key regulatory processes and key concerns for a substance are identified.

Concerns associated with substance characteristics are identified graphically with icons:

- **SVHC** – the substance has been identified as an SVHC and is in the candidate list for authorisation.
- **CMR** – the substance is indicated as a CMR by at least one notified classification and labelling (i.e. Carc 1a or 1b; Muta 1a or 1b; Repr 1a or 1b).
- **PBT** – the substance is indicated as PBT by at least one registrant (i.e. Is PBT / vPvB).

4.5.2. Regulations

Here an outline is given of the four regulations with which ECHA is concerned, with links to each regulatory process under which the substance is affected. It is proposed to display all regulations / regulatory processes and to grey out those which are not relevant to the substance in question. The registrations managed by ECHA are / will be:

- REACH – Registration, Evaluation, Authorisation & Restriction of Chemicals – Regulation (EC) No 1907/2006
- CLP – Classification, Labelling and Packaging of substances and mixtures – Regulation (EC) No 1272/2008
- BPR – Biocidal Product Regulation – Regulation (EU) 528/2012
- PIC – Prior Informed Consent Regulation – Regulation (EU) 649/2012

4.5.2.1. REACH

Identified processes to be included are:

- Registration
  - Pre-registration – indicated if substance EC / List number is found in the list of pre-registered substances.
  - Registration – indicated if there are registered dossiers for the substance.
- Evaluation
  - Dossier evaluation – indicated if one or more registered dossier for the substance has been evaluated under REACH and associated decision(s) published on the ECHA website.
  - Substance evaluation – indicated if substance EC / List number appears in the CoRAP list.

- Authorisation
  - Candidate List – indicates if the substance EC / List number is found in the candidate list.
  - Annex XIV (Authorisation List) – indicates if the substance EC / List number is found in the authorisation list.
- Restriction
  - Annex XVII (List of restrictions) – indicates if the substance EC / List number is found in the list of restrictions.

Table 5 – REACH

REACH Regulatory Actions for a substance			
Regulatory process / list	**Substance link**	**Displayed text**	**Link 3rd Tier**
Pre-registration	If EC / List no. present in pre-registration list	This substance has been pre-registered under REACH.	Pre-registration list entry
Registration	If registered dossier(s)	This substance has been registered under REACH.	Relevant dossier(s)
Dossier Evaluation	If there are dossiers evaluation decisions published for the substance	Registration dossiers for this substance submitted to ECHA have been evaluated under REACH.	Relevant evaluation decision(s)
Substance Evaluation	If EC / List no. present in CoRAP list	This substance is being evaluated under the Community Rolling Action Plan (CoRAP).	CoRAP list entry
Candidate List	If EC / List no. present in candidate list	This substance has been identified as a substance of very high concern (SVHC) and is a candidate for authorisation.	Candidate list for authorisation entry
Annex XIV (Authorisation List)	If EC / List no. present in authorisation list	According to Annex XIV of REACH this is a substance of very high concern and requires authorisation before it is used.	Authorisation list entry
Annex XVII (Restriction List)	If EC / List no. present in restriction list	Some uses of this substance are restricted under Annex XVII of REACH	Restriction list entry(ies)

4.5.2.2. CLP

Identified processes to be included are:

- Harmonisation – indicates if a harmonised entry exists for the substance.
- Notification – indicates that notified C&L's have been submitted to ECHA for a substance.

Table 6 – CLP

CLP Regulatory Actions for a substance			
Regulatory process / list	**Substance link**	**Displayed text**	**Link 3rd Tier**
Harmonisation	If harmonised entry exists for substance (i.e. if Index number is not blank)	A European Union Harmonised Classification & Labelling has been assigned to this substance	C&L Inventory harmonised entry
Notification	If notified C&Ls exist for the substance	Classification & Labellings have been notified to ECHA by Industry for this substance	C&L Inventory notified entries

4.5.2.3. BPR

Identified processes to be included are:

- Approval – indicates if the substance is an approved Biocidal Active Substance.
- Authorisation – indicates if there exist authorised Biocidal Products which use this substance as active ingredient.

Table 7 – BPR

BPR Regulatory Actions for a substance			
Regulatory process / list	**Substance link**	**Displayed text**	**Link 3rd Tier**
Approval	If substance EC / List number appears in approved AS list	This substance is approved for use as a Biocidal Active Substance	BAS entry / entries; potentially also Art 95(2) AS datasets (to be discussed)
Authorisation	If substance is an AS and if there exist authorised BPs using it as active ingredient	There are authorised Biocidal Products that use this substance as an active ingredient	BP entries

4.5.2.4. PIC

Identified processes to be included are:

- Annex I – indicates if the substance subject to PIC.
- Annex V – indicates if the substance is prohibited from export.

Table 8 – PIC

PIC Regulatory Actions for a substance			
Regulatory process / list	**Substance link**	**Displayed text**	**Link 3rd Tier**
Annex I	If substance EC / List number appears	This substance is subject to the Prior Informed Consent (PIC) regulation (Regulation (EU) 649/2012) and cannot be exported without notifying ECHA	(tbd); PIC annex I list entry
Annex V	If substance EC / List number appears	This substance is subject to the Prior Informed Consent regulation and is prohibited from export due to its hazardousness	(tbd) ; PIC annex V list entry

4.6. About this substance

This section gives an overview of the substance, the volume which is manufactured or imported to the EEA, what it is used for, how citizens and workers are likely to be exposed to it, and how manufacturers have informed ECHA the substance is to be used safely.

4.6.1. Volume of the substance

The volume calculation is based on the current tonnage band dissemination logic. The only difference is that under the substance centric approach the algorithm would take as input **ALL** registrations for a substance. The resulting output tonnage band would be relevant to all of the data ECHA holds on a substance (and would for instance result in merging data from joint and individual submissions for the same substance).

An additional logic would frame the output tonnage band in an appropriate text:

- No data (i.e. not registered) => This substance has not been registered under the REACH Regulation, therefore as yet ECHA has no usable data available about this substance.
- [Confidential] => This substance is manufactured and/or imported in the European Economic Area.
- Intermediate use only => This substance is manufactured and/or imported in the European Economic Area but is used up in the production of other chemical substance(s).
- Open or closed tonnage band => This substance is a [High / Medium / Low] production volume chemical; per year [Tonnage Band] tonnes are manufactured and / or imported in the European Economic Area.

4.6.2. Use Descriptors Logic Summary

1. Start with frame text for Product Category – "This substance is used in products such as:"
2. Count submitted non-confidential occurrences of Product Category use descriptors.
3. Remove outlier(s)
4. Rank by number of occurrences
5. Display user friendly text per use descriptor code in rank order.

The same approach is used for Sector of end use (SU), Process Category (PROC), and Environmental Release Category (ERC) codes. The result is a brief paragraph per use descriptor code type.

4.6.3. Precautions and safe use

This section will be linked to the precautions and / or guidance on safe use in the various registered dossier(s) for the substance.

4.7. Physical & Chemical Properties

This section will summarise physical & chemical property data from all registered dossiers for the substance.

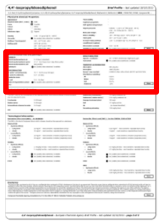
Key endpoints have been identified and included based on known chemical databases.

For each endpoint a title identifies the datum. An icon (if applicable) highlights key information (e.g. flammable, has an odour, no usable data provided to ECHA etc.). The experimental result is presented as a range min – max value in ECHA's database, at experimental conditions (also presented as a range). E.g. Octanol-Water Partition 2.20 – 3.32 LogKow (@ 20.0 – 21.5 °C and pH 3 – 6.7).

To calculate the ranges units and data are normalised wherever possible.

'More' links to the registered dossier(s) for the substance.

4.8. Environmental Fate and Pathways



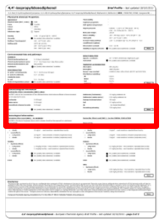
This section will summarise environmental property data from all registered dossiers for the substance.

Key endpoints have been identified and included.

Endpoint data is summarised as above.

'More' links to the registered dossier(s) for the substance.

4.9. Ecotoxicological Information



This section will summarise PNEC values for the substance.

The PNEC data is to be summarised using the same treatment as described above.

'More' links to the registered dossier(s) for the substance

4.10. Toxicological Information

This section will summarise DNEL values for the substance.

The DNEL data is to be summarised using the same treatment as described above.

'More' links to the registered dossier(s) for the substance

4.11. Disclaimer

Suitable legal disclaimer text specific to the brief profile and in addition to the general ECHA website legal disclaimer.

5. Infocard

The Infocard is proposed to be a simple high-level summary of information held by ECHA on a substance. This would be designed to be understandable to the broadest possible audience and to contain the most relevant data for the audience. The vision of how these would appear is that whenever a list of substance search results is displayed on the ECHA website, each row would be expandable into an Infocard for the relevant substance.

5.1. Header

The header of the Infocard is identical to that of the Brief Profile and will contain the ECHA Substance Name and the last updated date of the Infocard. It is also proposed to show synonyms in a second line, in alphabetical order, truncating those which do not fit and displaying only on mouse-over.

5.2. Substance Identity Block

This block will allow identification of a substance and it is to be populated from data contained in the proposed ECHA Substance Master List. It will contain the most basic non-confidential substance identifying data, such as:

- Numerical identifiers – EC and CAS numbers
- The substance molecular formula (if possible)
- A molecular structure image generated from the master list data (if possible)

5.3. Safety Classification and Labelling

This section is designed to provide a user friendly summary interpretation of the classification and labelling of the substance. It will be derived from the presentation shown in the brief profile but will show only:

- EU Harmonised Classification & Labelling – if extant, otherwise
- Notified Classifications & Labellings – derived from all classifications and labellings notified to ECHA, otherwise
- There is no harmonised classification and there are no notified hazards for this substance.

5.4. Summary of Concerns

This section summarises key concerns for a substance and the key regulatory actions which affect the substance. It is summarised from the content displayed in the Brief profile and will again show an icon for SVHC, CMR or PBT substances, and simple textual descriptions of identified key regulatory processes.

5.5. About this substance

This block is summarised from the data shown in the Brief Profile and gives an overview of the substance, the volume which is manufactured or imported to the EEA, what it is used for, and how citizens are likely to be exposed.

In the Infocard the (industrial) Processes in which the substance is used are omitted, as these are not likely to be routes via which the general public is exposed to the substance.

6. Annex – Example (Bisphenol-A)

6.1. Infocard

4,4'-isopropylidenediphenol DRAFT ***Infocard*** *– last updated 18/10/2013*

2,2-bis (4-hydroxyphenol) propane; 2,2-di(4-hydroxyphenyl)propane; 4,4' isopropylidinediphenol; Biphenol A; Bisferol A; **BPA**; C006780; DIAN; Ipognox 88; ...

Substance Identity
EC Number 201-245-8
CAS Number 80-05-7
Molecular Formula C15H16O2

HO OH

Safety classification & labelling

Caution! This substance can be very hazardous. This substance causes serious eye damage, is suspected of damaging fertility, may cause respiratory irritation, may cause an allergic skin reaction.
The above is based on a European Union Harmonised Classification & Labelling

Summary of Concerns and Regulations
There are at present no known concerns relating to this substance.

It is being evaluated under the CoRAP programme.
It is a candidate for restriction.
It has been analysed and a harmonised classification assigned.

About this substance
This substance is a High Production Volume (HPV) chemical; per year 1,000,000+ tonnes are made in or imported into the European Economic Area.

This substance is used in products or processes such chemical processing in order to be transformed into another substance (use of intermediates), coatings, paints, paint thinners & removers, fillers, putties, plasters, modelling clay, adhesives, sealants, polymers.

This substance is used in fields such as plastic product manufacture, mixing and/or re-packaging, computer, electrical, electronic and optical product manufacture, building & construction work, manufacture of machinery, equipment, vehicles & other transport equipment, pulp, paper and paper product manufacture, electricity, steam, gas, water supply and sewage treatment, rubber product manufacture.

Release to the environment of this substance is likely to occur from indoor use in long-life articles with low release, industrial use (in finished products), formulation, outdoor use in long-life articles with low release, industrial use as an intermediate step in further manufacturing, formulation, indoor use resulting in spreading of the substance, outdoor use resulting in spreading of the substance, manufacturing, industrial use for thermoplastic manufacture.

Precautions and Safe Use
Precautions suggested by manufacturers and importers of this substance can be found here; guidance provided by manufacturers and importers on the safe use of the substance can be found here.

More

4,4'-isopropylidenediphenol - European Chemicals Agency Infocard - last updated 18/10/2013

6.2. Brief Profile

4,4'-isopropylidenediphenol

DRAFT

***Brief Profile** – last updated 18/10/2013*

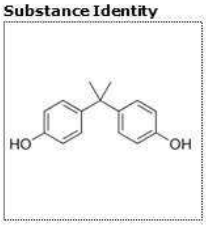
2,2-bis (4-hydroxyphenol) propane; 2,2-di(4-hydroxyphenyl)propane; 4,4' isopropylidinediphenol; Biphenol A; Bisferol A; **BPA**; C006780; DIAN; Ipognox 88; ...

Introduction

The following is a brief profile summarising the non-confidential data on this substance held in the databases of the European Chemicals Agency (ECHA). Please note that this brief profile is generated automatically based on the data available at the time of generation. The data remains the responsibility of its respective owners and ECHA does not assure the quality and correctness of the information. This brief profile is covered by the ECHA Legal Disclaimer.

More

Substance Identity



EC Number	201-245-8	**Type of Substance**	Mono constituent substance
EC Name	4,4'-isopropylidenediphenol	**Origin**	Organic
CAS Number	80-05-7		
Index Number	604-030-00-0	**Registered Compositions**	7
Molecular Formula	C15H16O2		
IUPAC Name	2,2-bis (4-hydroxyphenol) propane	**Of which contain:**	
Other Names	2,2-bis (4-hydroxyphenol) propane; 2,2-di(4-hydroxyphenyl)propane; 4,4' isopropylidinediphenol;	***Impurities relevant for classification***	2 compositions
		Additives relevant for classification	No compositions
Smiles	Oc1ccc(cc1)C(c2ccc(O)cc2)(C)C		
InChI	1S/C15H16O2/c1-15(2,11-3-7-13(16)8-4-11)12-5-9-14(17)10-6-12/h3-10,16-17H,1-2H3	**Substance Listed**	EINECS (European Inventory of Existing Commercial Chemical Substances)

More

Safety Classification & Labelling

EU Harmonised Classification & Labelling (ATP 4 – Sep 2013)

Caution! This substance can be very hazardous. This substance causes serious eye damage, is suspected of damaging fertility, may cause respiratory irritation, may cause an allergic skin reaction.

More

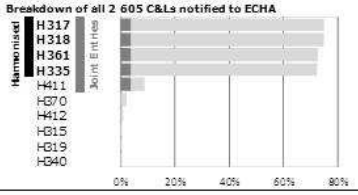
Notified Classifications & Labellings

Caution! This substance can be very hazardous. This substance causes serious eye damage, is suspected of damaging fertility, may cause respiratory irritation, may cause an allergic skin reaction.

The above is compiled based on all of the classifications and labellings notified to ECHA by industry

More

Breakdown of all 2 605 C&Ls notified to ECHA



Concerns & Regulations / Regulatory Action on this substance

Summary of Concerns

There are at present no concerns relating to this substance.

Registration, Evaluation, Authorisation & Restriction of Chemicals (REACH)

Registration
Pre-registration *Indication by companies that the substance would be registered*
Registration *Submission of dossier of information on a substance*

Evaluation
Dossier Evaluation *Indication that one or more dossiers submitted to ECHA to register this substance have been evaluated under REACH*
Substance Evaluation *Indication that this substance is being evaluated under the Community Rolling Action Plan (CoRAP)*

Authorisation
Candidate List *Indication that this substance has been identified as a substance of very high concern (SVHC) and is a candidate for authorisation*
Annex XIV (Authorisation List) *Indication that according to Annex XIV of REACH this substance is an SVHC and that it requires authorisation before it can be used*

Restriction
Annex XVII (Restriction List) *Indication that some uses of this substance are restricted under Annex XVII of REACH*

Classification Labelling & Packaging (CLP)

Harmonised C&L *Indication that a European Union harmonised classification and labelling has been assigned to this substance*
Notification *Indication that industry has notified ECHA of classifications and labellings for this substance*

Biocidal Products Regulation (BPR)

Active Substance *Indication that this substance is approved for use as a Biocidal Active Substance*
Biocidal Products *Indication that there are authorised biocidal products that use this substance as an active ingredient*

Prior Informed Consent (PIC)

Annex I *Indication that this substance is subject to the PIC regulation and cannot be exported from the EEA without informing ECHA*
Annex V *Indication that this substance is subject to the PIC regulation and is prohibited from export due to its hazardousness*

About this substance

General
This substance is a High Production Volume (HPV) chemical; per year 1,000,000+ tonnes are made in or imported into the European Economic Area.

Product Categories
This substance is used in products or processes such as chemical processing in order to be transformed into another substance (use of intermediates), coatings, paints, paint thinners & removers, fillers, putties, plasters, modelling clay, adhesives, sealants, polymers.

Sectors of use
This substance is used in fields such as plastic product manufacture, mixing and/or re-packaging, computer, electrical, electronic and optical product manufacture, building & construction work, manufacture of machinery, equipment, vehicles & other transport equipment, pulp, paper and paper product manufacture, electricity, steam, gas, water supply and sewage treatment, rubber product manufacture.

Processes in which used
This substance is used in activities or processes at workplace such as transfer (large), at dedicated facilities, closed batch processing, closed process with occasional exposure, transfer (small), batch processing, batch and other processing, production by tabletting, compression, extrusion or pelletisation, roller or brush application, treatment by dipping and pouring, transfer (large), non-dedicated facilities.

Environmental Release & Exposure
Release to the environment of this substance is likely to occur from indoor use in long-life articles with low release, industrial use (in finished products), formulation, outdoor use in long-life articles with low release, industrial use as an intermediate step in further manufacturing, formulation, indoor use resulting in spreading of the substance, outdoor use resulting in spreading of the substance, manufacturing, industrial use for thermoplastic manufacture.

Precautions and Safe Use
Precautions suggested by manufacturers and importers of this substance can be found here; guidance provided by manufacturers and importers on the safe use of the substance can be found here.

More

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4,4'-isopropylidenediphenol** – European Chemicals Agency Brief Profile – last updated 18/10/2013 – **page 1 of 2

4,4'-isopropylidenediphenol

DRAFT

***Brief Profile** – last updated 18/10/2013*

2,2-bis (4-hydroxyphenol) propane; 2,2-di(4-hydroxyphenyl)propane; 4,4' isopropylidinediphenol; Biphenol A; Bisferol A; **BPA**; C006780; DIAN; Ipognox 88; ...

Physical & Chemical Properties

Appearance

Physical state (20°C, 1 atm)	Solid
Form	Crystals
Colour	White
Odour	Odourless
Substance type	Organic
Density	1.06 – 1.2 g/cm³ (@ 20 – 160°C)
Viscosity	No (usable) data submitted / available
Melting / freezing point	150 – 157°C (@ 1 atm)
Boiling point	220°C @ 5.22 hPa 250 – 252°C (@ 17 hPa) 220 – 360°C (@ 1 atm)
Flammability	-
Explosive properties	-
Self-ignition temperature	-
Vapour pressure	0.00161 – 1.297 x 10⁻⁷ hPa (@ 20 – 50 °C) 0.09 – 10.13 hPa (@ 170 – 190°C)
Molecular weight	228.29
Water solubility	120 – 340 mg/L (@ 25 – 83°C and pH 4 – 10)
Flash point	207 – 227 °C (@ ~1 atm)
Octanol-water partition coefficient (LogKow)	2.20 – 3.32 logKow (@ ~21.5°C and pH 3 – 6.7)
Dissociation constant	9.73 – 10.48
Stability in organic solvents	No (usable) data submitted / available

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Environmental fate and pathways

STABILITY

Phototransformation in air	0.13 days (calculated)
Phototransformation in water	17.4 – 32.2 hours (river / lake fulvic acids)
Phototransformation in soil	No (usable) data submitted / available
Hydrolysis	Data waiving

BIODEGRADATION

In water: screening tests	74.7 – 81.4% (over 28 days)
In water & sediment: simulation tests	0.5 – 2.6 days
In soil	0.5 – 2.6 days
Mode of degradation (actual use)	No (usable) data submitted / available

BIOACCUMULATION

Aquatic / sediment	20 – 67 BCF (whole body weight @ 15 µg/l)
Terrestrial	No (usable) data submitted / available

TRANSPORT & DISTRIBUTION

Adsorption	890 L/kg Koc
Desorption	1090 L/kg Koc
Henry's Law constant	0.000312 other: mPa m³/mol (@ 25°C and 1013 hPa)
Distribution modelling:	
Air	0.01%
Water	32.9%
Soil	65.3%
Sediment	1.8%

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Ecotoxicological information

Predicted No-Effect Concentration (PNEC) values

The PNEC value is the concentration of the substance below which adverse effects in the environment are not expected to occur.

Freshwater	0.018 mg/L
Marine water	0.016 mg/L
Intermittent releases to water	0.01 mg/L
STP	No (usable) data submitted / available
Sediments (freshwater)	2.2 mg/kg sediment dw
Sediments (marine water)	0.44 mg/kg sediment dw
Sewage treatment plant	320 mg/L
Soil	3.7 mg/kg soil dw
Air	- (no hazard identified)
Secondary poisoning	13.8 mg/kg food

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Toxicological information

Derived No-Effect Level (DNEL) – for WORKERS

The DNEL is the level of exposure above which a human should not be exposed to a substance.

INHALATION

• **Systemic effects**	
○ **Long term**	10 mg/m³ – most sensitive: repeated dose toxicity
○ **Acute**	10 mg/m³ – most sensitive: repeated dose toxicity
• **Local effects**	
○ **Long term**	10 mg/m³ – most sensitive: irritation (respiratory tract)
○ **Acute**	10 mg/m³ – most sensitive: irritation (respiratory tract)

DERMAL

• **Systemic effects**	
○ **Long term**	1.4 mg/kg bw/day – most sensitive: repeated dose toxicity
○ **Acute**	1.4 mg/kg bw/day – most sensitive: repeated dose toxicity
• **Local effects**	
○ **Long term**	No (usable) data submitted / available
○ **Acute**	No (usable) data submitted / available

EYES No (usable) data submitted / available

Derived No-Effect Level (DNEL) – for the GENERAL POPULATION

INHALATION

• **Systemic effects**	
○ **Long term**	0.25 mg/m³ – most sensitive: repeated dose toxicity
○ **Acute**	5 mg/m³ – most sensitive: repeated dose toxicity
• **Local effects**	
○ **Long term**	5 mg/m³ – most sensitive: irritation (respiratory tract)
○ **Acute**	5 mg/m³ – most sensitive: irritation (respiratory tract)

DERMAL

• **Systemic effects**	
○ **Long term**	0.7 mg/kg bw/day – most sensitive: repeated dose toxicity
○ **Acute**	0.7 mg/kg bw/day – most sensitive: repeated dose toxicity
• **Local effects**	
○ **Long term**	No (usable) data submitted / available
○ **Acute**	No (usable) data submitted / available

EYES No (usable) data submitted / available

ORAL

• **Systemic effects**	
○ **Long term**	0.05 mg/kg bw/day – most sensitive: repeated dose toxicity
○ **Acute**	0.05 mg/kg bw/day – most sensitive: repeated dose toxicity

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