Environment Agency

Evidence

Environmental risk evaluation report: Styrenated phenol

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Miranda Kavanagh

Miranda Kavanagh

Director of Evidence

Executive summary

Styrenated phenol (CAS number 61788-44-1) belongs to a group of phenols which are used as antioxidants. These chemicals are of potential concern because they have widespread use, and can be highly toxic to aquatic organisms. In addition, styrenated phenol may be used as a replacement for substances of concern such as nonylphenol for some uses, for example as an intermediate for surfactants.

Styrenated phenol is used as an antioxidant in rubber, and as an intermediate in the production of surfactants (ethoxylates). These are used largely in the formulation of crop protection products, with minor uses as anti-static agents for wool and stabilisers for polyurethane foams. There are four current European Union (EU) producers of styrenated phenol and it is a high production volume chemical (over 1,000 tonnes per year).

Information for this assessment was collected through an online literature search (Chemical Abstracts) and through web searches. Further information was provided by manufacturers and users of the substance during consultation on drafts of the report in 2006, 2007 and 2008.

Styrenated phenol is made up of three main components; mono-, di- and tristyrenated phenol. The relative amounts of each component differ depending on the use of the substance. Styrenated phenol used to make surfactants has a typical tristyrenated component content of 70 per cent, with 23 per cent distyrenated and two per cent monostyrenated. Styrenated phenol used as an antioxidant has typically 43 per cent di- and tristyrenated phenol, with 11 per cent of the monostyrenated component. The components have notably different properties. For this assessment, the predicted environmental concentrations (PECs) of each component were calculated individually, and compared with predicted no-effect concentrations (PNECs) for each component.

Styrenated phenol is not readily biodegradable according to standard tests. There are some indications of degradation from related substances, and the substance would be expected to react with oxidants in the environment in view of its intended function; as a result, inherent degradability in the environment was assumed in the assessment. Styrenated phenol is expected to partition mainly to soil and sediment in the environment. Based on the predicted log K_{ow} value, monostyrenated phenol has a moderate bioaccumulation potential. A dietary fish bioaccumulation study has shown that tristyrenated phenol accumulates significantly, but that distyrenated phenol is not accumulative. Emission estimates are largely based on generic industry information and default values, with limited substance-specific information (relating to production and rubber production).

There is limited information on aquatic toxicity; short-term studies with fish and *Daphnia* where the exposure concentrations were above the solubility, and one valid long-term study on *Daphnia* for each of di- and tristyrenated phenol. Quantitative structure-activity relationship (QSAR) predictions of long-term toxicity were used with the measured data to derive aquatic fresh water PNEC values for each component: 21 µg/l for monostyrenated, 4.5 µg/l for distyrenated and 0.42 µg/l for tristyrenated. There are no toxicity data for sediment or soil organisms, so PNEC values for these were calculated from the PNEC for water. Worst case PNEC values for secondary poisoning were derived: 1.2 mg/kg for monostyrenated, and 4.8 mg/kg for di- and tristyrenated. A PNEC of 11.11 mg/kg is also used for a commercial product.

Based on available information and screening data, styrenated phenol meets the criteria for very bioaccumulative (vB), persistent (P) and possibly very persistent (vP) in the environment. It is not currently clear if styrenated phenol meets toxicity criteria due to lack of data.

No risks are identified for production of styrenated phenol. Potential risks are identified for the freshwater aquatic, marine aquatic and terrestrial environment for a number of life-cycle stages. These risks are largely due to the tristyrenated component. There are risks for all relevant stages for freshwater and marine sediments, and for the terrestrial food chain. There is a risk for marine predators in one scenario. There are no risks for wastewater treatment or for marine top predators. Risks to humans were not assessed.

Styrenated phenol is not produced in the United Kingdom (UK). It is supplied to the UK for use in the production of surfactants, and use in the UK in rubber is assumed. The priority for further investigation is the PBT (persistent, bioaccumulative and toxic) and vPvB (very persistent and very bioaccumulative) assessment. Testing on persistence is recommended; long-term testing on fish could be considered if persistence testing shows that the substance meets the persistent (P) but not vP criteria. As the predicted environmental concentrations rely heavily on generic or default values, specific data on actual emissions are needed, preferably based on measurements. For the sediment and soil assessments, toxicity testing on organisms may also be needed, but this will depend on the provision of better exposure information.

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- Conseil Européen des Phénols Alkylés et Derivés (European Council for Alkylphenols and Derivatives) (CEPAD)
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- Association of European Adhesives Manufacturers (FEICA)
- Lanxess
- Rhodia

who provided information for this report mainly through the Styrenated Phenol Task Force (SPTF) or via the Chemical Stakeholder Forum (CSF), and the Heath and Safety Executive (HSE) who provided the mammalian toxicity review.

Preface

The Environment Agency undertook a scoping exercise to prioritise further evaluation of environmental risks from alkyl and aryl phenols which could be considered as possible replacements for nonylphenol, including use of derivatives such as ethoxylates (Environment Agency, 2005a). The report indicated that styrenated phenol should be a priority for further work confirming an initial screen conducted previously (Environment Agency, 2002). Styrenated phenol is a substituted phenol used as a rubber antioxidant and as an intermediate in the production of surfactants used as additives in the formulation of agrochemicals. Styrenated phenol is reported to be produced at high volumes within the European Union (EU) and is used in a range of different products. As a consequence of its use and high volume production, there is potential for widespread release to the environment. This assessment is included in the United Kingdom Coordinated Chemicals Risk Management Programme (UKCCRMP)[1].

Styrenated phenol compounds

The initial scoping exercise (Environment Agency, 2005a) identified four styrenated phenol type compounds:

- Styrenated phenol (CAS number 61788-44-1).
- Tristyrylphenol (CAS number 18254-13-2).
- Isobutylated, methylstyrenated phenol (CAS number 68457-74-9).
- Distyrenated hydroxyl toluene (CAS number 1817-68-1).

The commercial products styrenated phenol and tristyrylphenol consist of a mixture of isomers of styryl-substituted phenol. Tristyrylphenol is characterised by a relatively high content of the tristyrenated isomer. These compounds exist as mixtures of components with different positions and levels of substitution, each of which can have different physicochemical characteristics. This has implications for how potential environmental risks posed by the compounds are assessed - these are discussed at the start of Section 1. The potential environmental risks of each group of isomers (mono-substituted, di-substituted and tri-substituted) are assessed separately. The final risk characterisation is based on the sum of the risks of these components.

Isobutylated, methylstyrenated phenol was categorised by the American Chemistry Council (ACC) as part of the ‘styrenated phenol’ category under the US HPV Challenge Programme (ACC, 2003). Distyrenated hydroxyl toluene derivative was listed in the UK Environment Agency’s prioritisation of alkyl and arylphenols report (Environment Agency, 2005a), but was not listed by the American Chemistry Council. These two styrenated phenols have been further described as part of a group of chemicals called hindered phenols, characterised by one or more *ortho*-substituted phenol groups (United States Environment Protection Agency (USEPA), 2002). Hindered phenols share similar characteristics with respect to physiochemical, environmental fate and ecotoxicological properties, although there is less agreement as to the nature of potential health effects (USEPA, 2002).

Information on the use of isobutylated, methylstyrenated phenol and distyrenated hydroxyl toluene is extremely limited. An internet search indicated distyrenated hydroxyl toluene may be an antioxidant in rubber or a surfactant component. However,

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[1] The UKCCRMP is a joint programme between Defra and the Environment Agency to consider hazard and risk assessment, and risk management of chemicals, in the period leading up to the first assessments under REACH (Regulation for the Registration, Evaluation, Authorisation and Restriction of Chemicals). Available from: http://www.defra.gov.uk/environment/chemicals/csf/criteria/index.htm.

this substance was not classified in Annex 1 of Directive 67/548/EEC and therefore is not harmonised in Regulation EC 1272/2008 on the Classification, Labelling and Packaging of Substances and Mixtures. It has not been reported as a high production volume chemical (HPVC) or a low production volume chemical (LPVC) on the ESIS (European Chemical Substances Information System) database, and IUCLID (International Uniform Chemical Information Database) or OECD (Organisation for Economic Cooperation and Development) Chemical Data Sheets are not available. The physicochemical characteristics and potential environmental effects of this compound can be predicted using the EPIWIN (Estimation Programs Interface Suite™) (v3.12) estimation software (USEPA, 2004). However, in the absence of any market information on possible uses and quantities, it is not appropriate to include this chemical in the assessment. A similar conclusion applies to the isobutylated, methylstyrenated phenol derivative, for which there is also little information available.

The assessment focuses on styrenated phenol (CAS number 61788-44-1) and tristyrylphenol (CAS number 18254-13-2), for which information on usage is available. The purpose of this report is to identify the properties of this chemical that might lead to environmental or human health concerns. It also investigates points in the chemical's life-cycle where risks might occur. The assessment is for the environment only, and does not consider human health risks. The information will be used by the Chemicals Policy function of the Environment Agency and the Department for Environment, Food and Rural Affairs (Defra) to inform risk management decisions and will also be useful for industry in identifying areas which may need further work for chemical safety assessments under REACH (Regulation for the Registration, Evaluation, Authorisation and Restriction of Chemicals). This and the other reports in this series are not intended to provide a basis to decide whether a substance is suitable for a particular purpose.

The data collection and peer-review for this report are described in Appendix 1. Data were reviewed according to the EU Technical Guidance Document (TGD) (EC, 2003).

The layout follows the format of an Exisiting Substances Regulation (ESR)[2] assessment with a few small modifications, so that readers familiar with such assessments (for example, those for bisphenol-A and nonylphenol) can quickly find the information they are interested in.

The substance is not manufactured in the UK. The assessment has relied on the voluntary provision of data from industry. Information on uses and supply levels is only available at the European level. However, given the nature of the open market in Europe, the assessment assumes that any use of the substance at the European level could take place in the UK, unless there is reliable evidence to suggest that this is not the case (for example, if only a small number of non-UK locations are known to use a particular process).

This report is supported by a confidential annex containing commercially sensitive information not for the public domain.

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[2] Regulation EEC 793/93 on the Evaluation and Control fo the Risks of Existing Substances

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1 General substance information

This study assesses the potential environmental risk from styrenated phenol (CAS number 61788-44-1) and tristyrylphenol (CAS number 18254-13-2). Both commercial products exist as a mixture of isomers. Three isomers exist of the monostyrenated form, two of the distyrenated and one of the tristyrenated forms. For the purposes of this report, the term 'component' is used to refer to each group of isomers[3], and the term 'compound' is used to describe the whole mixture of isomers that make up the commercial product.

According to information provided by the Styrenated Phenol Task Force (SPTF), the ratio of components within a commercial compound varies according to the intended use of that compound. The monostyrenated phenol component accounts for 0-15 per cent of a commercial compound. The distyrenated phenol component accounts for 10-52 per cent, and the tristyrenated phenol component for 40-80 per cent (SPTF, 2006).

Due to differences in the physicochemical characteristics of the three components in the commercial products, any styrenated phenol or tristyrylphenol released to the environment will not behave as a single compound. Significant variation is expected in the fate, behaviour and toxicity of the three components. As a consequence, it was considered more appropriate to conduct the environmental risk assessment for the three components of the commercial products, rather than for the mixture. Therefore, for the most part this assessment calculates separate PEC/PNEC (predicted environmental concentration/predicted no-effect concentration) ratios for each component; monostyrenated, distyrenated and tristyrenated phenol.

There are also differences in the physicochemical characteristics (and therefore the fate and behaviour) of individual isomers of each component, particularly the distyrenated phenol isomers. Such differences are considered in the assessment as follows:

- Monostyrenated component. Quantitative structure-activity relationship (QSAR) predictions of physicochemical properties of the three isomers of the monostyrenated component are sufficiently similar not to affect the environmental risk assessment. They are treated as one component.
- Distyrenated component. The physicochemical characteristics of the two isomers of the distyrenated component are sufficiently different to warrant consideration in the assessment. The two isomers, 2,4-distyrenated phenol (15-25 per cent of the technical product) and 2,6-distyrenated phenol (20-30 per cent of the technical product) are present at a ratio of 4:5 (Herdillia, 2005).
- Tristyrenated component. There is only one isomer of the tristyrenated phenol component.

To facilitate the three-component approach, an indicative composition of the commercial product was agreed with industry for the purposes of the risk assessment. Because different applications of styrenated phenol use products with different ratios of the three components, the risk assessment process was conducted with representative formulations (described in the bullet points below).

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[3] The terms 'monostyrenated', 'distyrenated' and 'tristyrenated phenol' are also used as generic terms for the group of isomers that exist for that particular component.

The formulations that were assessed are[4]:

- Commercial product A (representative of the styrenated phenol used as an antioxidant in rubber) (Lanxess, personal communication, 2005):
  - monostyrenated phenol, 11 per cent;
  - distyrenated phenol, 43 per cent;
  - tristyrenated phenol, 43 per cent.
- Commercial product B (representative of the styrenated phenol used in the production of some styrenated phenol ethoxylates) (Cognis, personal communication, 2005).
  - monostyrenated phenol, 2 per cent;
  - distyrenated phenol, 23 per cent;
  - tristyrenated phenol, 70 per cent.

A similar composition of monostyrenated phenol 2.5 per cent, distyrenated phenol 25 per cent, and tristyrenated phenol 70 per cent was reported for styrenated phenol produced for use in ethoxylates (SPTF, 2007).The composition of the tristyrenated phenol commercial product is similar to that of commercial product B.

The remaining content of the commercial products (three per cent for product A and five per cent for product B) is assumed to be impurities (see Section 1.2.1)

Predicted no-effect concentrations (PNECs) were calculated for each of the three components in most cases. Predicted environmental concentrations (PECs) for each of the three components take account of which application uses which commercial product, and also the composition of the three components within that commercial product. The PEC/PNEC ratios of each component are summed to produce a single PEC/PNEC ratio for styrenated phenol.

1.1 Identification of the substance

1.1.1 Styrenated phenol

CAS number:	61788-44-1 (may also be referred to under the former CAS registry number 9010-16-6 (USEPA, 2006)[5]).	
EINECS number:	262-975-0	
EINECS name:	Phenol, styrenated	
Molecular formula:	$C_{14}H_{14}O$	(monostyrenated phenol)
	$C_{22}H_{22}O$	(distyrenated phenol)
	$C_{30}H_{30}O$	(tristyrenated phenol)

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[4] A complete list of the applications for commercial products one and two are given in Table 2.1.

[5] The CAS number 9010-16-6 is a Registry Number (RN) that has been deleted with the chemical styrenated phenol reassigned to the new RN 61788-44-1. No suppliers of a chemical with CAS number 9010-16-6 have been identified.

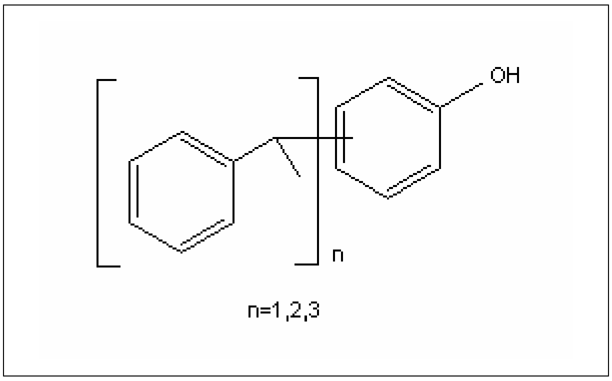

Figure 1.1 Structure of styrenated phenol (ACC, 2003).

Molecular weights were calculated using EPIWIN (v3.12) (USEPA, 2004).

SMILES (Simplified Molecular Input Line Entry System) codes[6]:

- Monostyrenated component:
  - **c1(O)c(C(C)c2ccccc2)cccc1**. SMILES code for the monostyrenated phenol (n=1 in Figure 1.1, with the styrenated subgroup in the *ortho* position). CAS number 4237-94-1. Molecular weight: 198.27.
  - **c1(O)ccc(C(C)c2ccccc2)cc1**. SMILES code for the monostyrenated phenol (n=1 in Figure 1.1, with the styrenated subgroup in the *para* position). CAS number 1988-89-2. Molecular weight: 198.27.
- Distyrenated component:
  - **c1(O)c(C(C)c2ccccc2)cc(C(C)c3ccccc3)cc1**. SMILES code for the 2,4-distyrenated phenol isomer (Figure 1.2). CAS number 2769-94-0. Molecular weight: 302.42.
  - **c1(C(C)c3ccccc3)c(O)c(C(C)c2ccccc2)ccc1**. SMILES code for the 2,6-distyrenated phenol isomer (Figure 1.3). CAS number not located. Molecular weight: 302.42.
- Tristyrenated component:
  - **c(ccc1C(-c(cc(c2O)C(-c(ccc3)cc3)C)cc2C(-c(ccc4)cc4)C)C)cc1**. SMILES code for the tristyrenated phenol (n=3 in Figure 1.1, 2,4,6-tristyrenated isomer). Molecular weight: 406.57. The commercial product (CAS number 18254-13-2) consists predominantly of the tristyrenated component, although it does contain small amounts of the monostyrenated and distyrenated components.

The following molecular weights for commercial products were reported in the literature:

- 322 g/mol (typical value; USEPA, 2003);
- 330 g/mol (average value; ACC, 2003);
- 367 g/mol (industry data; Tech Direct, 2005).

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[6] There are a range of possible correct SMILES codes for an individual structure; these are examples. Note also that the SMILES code in EPIWIN for the CAS number 6788-44-1 is not correct for any of the components.

Other names, abbreviations and trade names include the following:

Anox G2*
Kumanox SP
Lowinox P24S*
Mixed styrenated phenols
Montaclere S*
Montaclere SE*
Naugard SP
Phenol styrenated
Phenol styrolisiert
Prodox 120
SP, SPH
Styrenated phenol
Styrenated phenols
Vulcanox SP
Vulkanox
Vanox 102
Wingstay F93, S
Westco 120

*Styrenated phenols with these synonyms are reported in the literature, but are no longer available. They are listed here for historical reasons and completeness.

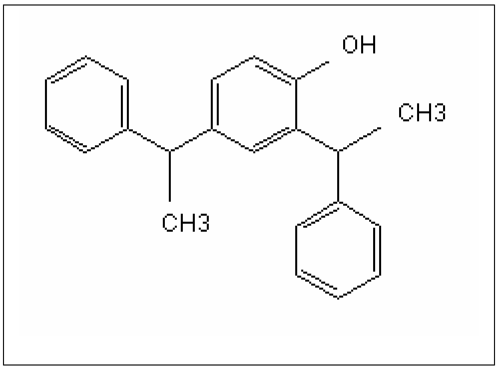


Figure 1.2 2,4-distyrenated phenol isomer.

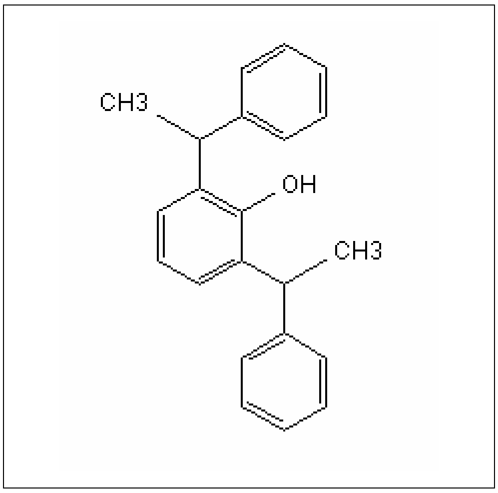


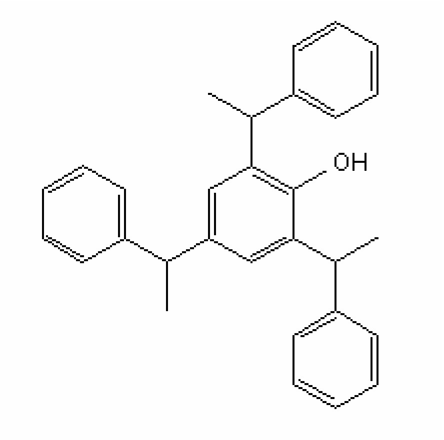
Figure 1.3 2,6-distyrenated phenol isomer.

1.1.2 Tristyrylphenol

CAS number:	18254-13-2
EINECS number:	242-128-1
EINECS name:	2,4,6-tris(1-phenylethyl)phenol

Molecular formula: $C_{30}H_{30}O$

Structural formula:



SMILES code: see the tristyrenated component in Section 1.1.1

Synonyms: Phenol, 2,4,6-tris(1-phenylethyl)
Tristyrenated phenol

Molecular weight: 406.57 g/mol

1.2 Purity/impurities, additives

1.2.1 Purity/impurities

Phenol is present in styrenated phenol (residual from the starting substance phenol) at a level of less than one per cent (Lanxess, personal communication, 2005).

The commercial product Wingstay F93 has a purity of 95 per cent (Tech Direct, 2005). The commercial product Wingstay S is reported to contain styrene dimer (under one per cent), styrene (0.05 per cent) and phenol (under one per cent), with the remaining product consisting of monostyrenated phenol (11 per cent), distyrenated phenol (43 per cent) and tristyrenated phenol (43 per cent) (Eliokem, personal communication, 2006). The composition of this product is typical of a generic styrenated phenol used as an antioxidant in rubber and is summarised in Table 1.1.

Table 1.1 Purity of the commercial product Wingstay S.

Component	Typical composition (%)	Range
Monostyrenated phenol	11.0	≤15%
Distyrenated phenol	43.0	40-52%
Tristyrenated phenol	43.0	40-46%
Styrene dimer	0.2	1,000-2,500 ppm
Styrene	0.5	100-1,000 ppm
Phenol	<1.0	5,000-10,000 ppm

1.2.2 Additives

There are no reported additives for the production of styrenated phenol.

1.3 Physicochemical properties

The following section provides a summary of the chemical and physical properties of styrenated phenol (the commercial mixture), and where available, for the individual components. The physicochemical properties of the individual components of styrenated phenol were estimated using the EPWIN v3.12 computer estimation software (USEPA, 2004). Full details of these calculations are given in Appendix 2. The physicochemical data used in the risk assessment is summarised in Table 1.2 at the end of the section.

With the exception of the water solubility and partition coefficient studies, only short summaries of the physicochemical tests from USEPA (2003) were reviewed for this assessment.

Klimisch codes are included for experimental results; all predicted values included here are considered to be Klimisch code 2 (valid with restrictions) unless otherwise noted.

1.3.1 Physical state (at normal temperature and pressure)

At normal temperature and pressure, styrenated phenol is a clear pale yellow to amber coloured liquid (USEPA, 2003).

1.3.2 Melting point

The melting point of styrenated phenol has been reported as below 0°C (no method specified, considered to be Klimisch code 2) (USEPA, 2003). IUCLID (2001) lists melting points for styrenated phenol of 25.82°C (determined by calculation) and below 0°C. No explanation of the difference between the two values is reported, but as the commercial products are liquids at room temperature the higher value may relate to a pure component. These studies cannot be assessed for reliability (Klimisch code 4).

1.3.3 Boiling point

The boiling point value for styrenated phenol has been reported as 230°C at 1,013 hPa pressure (USEPA, 2003, considered Klimisch code 2). No method was reported for the derivation of this value. IUCLID (2001) lists boiling points for styrenated phenol as 209.22°C (calculated value), 230°C (no method provided), and 200-250°C (no method provided); these results are all Klimisch code 4.

1.3.4 Relative density

The relative density for styrenated phenol has been reported as 1.08 at 20°C. This value was determined using the hydrometer method with standards set in ASTM-E-100 (ASTM D891-94) (USEPA, 2003, considered Klimisch code 1).

1.3.5 Vapour pressure

A calculated vapour pressure of styrenated phenol of 0.04413 hPa (0.0331 mm Hg, 4.41 Pa) at 25°C has been reported (USEPA, 2003). This appears to be very high for a substance of this structure. The same value can be calculated using EPIWIN (USEPA, 2004) with a boiling point of 230°C based on the SMILES code obtained when entering the CAS number 61788-44-1. As noted in Section 1.1.1, this SMILES code is incorrect and relates to a much smaller molecule.

The vapour pressure of the three individual components was determined by the modified Grain estimation method within the EPIWIN estimation software (USEPA, 2004) using the SMILES codes from Section 1.1:

- Monostyrenated phenol 4.9×10^{-5} mmHg at 25°C (6.53×10^{-3} Pa).
- Distyrenated phenol 1.93×10^{-8} mmHg at 25°C (2.57×10^{-6} Pa).
- Tristyrenated phenol 6.52×10^{-12} mmHg at 25°C (8.69×10^{-10} Pa).

The value above for distyrenated phenol applies to both isomers. There is some uncertainty in these values, but they are considered suitable for use in the assessment, as the methods used to estimate emissions and concentrations are not very sensitive to changes in the vapour pressure, especially for values as low as those for di- and tristyrenated phenol.

1.3.6 Water solubility

The water solubility of styrenated phenol is reported to be 59 mg/l at 20°C (measured value) (IUCLID, 2000). The same value is quoted by industry, along with the following information – the combined saturation concentration of mono-phenylethylphenols and phenol in a column experiment was 59 mg/l (ratio not reported). Di-or higher phenylethylphenol isomers were not found in the gas chromatogram (GC) of the eluate and the detection limit was not reported. No further details of the study are given and it is considered to be of only limited value (Lanxess, personal communication, 2005). It is not used in the assessment.

The water solubility for the commercial product Vulkanox SP is reported as 59 mg/l in an unpublished study report by Bayer AG and the value given in IUCLID (2000) is taken from this report (SPTF, 2007).

Water solubilities of the three individual components were determined by the slow stirring method at 20°C according to OECD 105 and EC 92/69 Method A.6 (Lange, 2005a, 2005b and 2005c). These measured values are given below:

- Monostyrenated phenol 231 mg/l at pH 6.63 (Lange, 2005a).
- Distyrenated phenol 0.665 mg/l at pH 6.96 (Lange, 2005b).
- Tristyrenated phenol below 0.025 mg/l at pH 6.51 (Lange, 2005c).

The purity of each test substance was reported (95 per cent for monostyrenated phenol, 97 per cent for distyrenated phenol and 95 per cent for tristyrenated phenol) (Lange, 2005a, 2005b and 2005c). The composition of distyrenated phenol and the ratio of 2,4- and 2,6-distryrenated phenol isomers was not given in the test report. Similarly the percentages of *ortho*- and *para*-monostyrenated phenol in the test substance were not reported. It is therefore not clear whether the analytical method measured the individual isomers. The results for the mono-and distyrenated phenols are considered to be valid and suitable for use in the assessment (Klimisch code 1).

The water solubility of tristyrenated phenol was determined using a column elution according to OECD 105 and EC 92/69 Method A.6 (Lange, 2008a). The purity of the substance used was 96 per cent. The initial flow through the column was discarded to remove water soluble impurities, the column was equilibrated overnight, and samples were taken until five successive samples showed variation of no more than 30 per cent. Two runs were conducted, one at half the flow rate of the other. Samples were checked for the presence of colloidal material, which was not found. The pH of the water was 7-8. The result was 7.1 µg/l. This study is considered valid (Klimisch code 1).

For comparison, the water solubilities of the three components were estimated using the EPIWIN program (USEPA, 2004). This has two models: WSKOW, which uses the estimated log K_{ow} as the basis for the value, and WATERNT which uses a fragment method based on structure. Predictions were also obtained using the WS_Multicase program within the OECD (Q)SAR toolbox (OECD, 2008). The results are given in Table 1.2, along with the measured values.

Table 1.2 Predicted and measured water solubility values (mg/l).

	WSKOW	WATERNT	Multicase	Measured
Monostyrenated phenol	125	52	37	231
2,4-Distyrenated phenol	0.48	0.0042	0.032	0.665
2,6- Distyrenated phenol	2.5	0.0042	0.023	0.665
Tristyrenated phenol	0.0086	3×10^{-5}	3.0×10^{-4}	0.0071

The predictions for the mono-, 2,4-di- and tristyrenated substances from WSKOW are close to the measured values. Those from WATERNT and Multicase are all below the measured values and in some cases over an order of magnitude lower.

The measured values were used in the assessment.

1.3.7 n-Octanol-water partition coefficient

A number of log K_{ow} values for styrenated phenol have been reported. The log K_{ow} value for styrenated phenol as a mixture and for the three components individually can vary with pH, although data are not currently available for this to be addressed here.

A log K_{ow} of 2.41 is reported in IUCLID (2001). The same value is calculated when CAS number 61788-44-1 is entered into EPIWIN. However, the SMILES code generated from this CAS number is incorrect and the compound identified is a much smaller molecule. Therefore this value of log K_{ow} is incorrect. A measured log K_{ow} value above four at 22°C is given in IUCLID (2000) (Klimisch code 4).

Lange (2007) determined a log K_{ow} of 6.24 at 25°C for distyrenated phenol using the slow stirring method according to OECD Guideline 123, 2006. The purity of the test substance was 99 per cent distyrenated phenol, consisting of 54 per cent 2,6-

distyrenated phenol and 45 per cent 2,4-distyrenated phenol. This study is considered valid (Klimisch code 1).

The same author (Lange, 2008b) determined a log K_{ow} value of 7.77 for tristyrenated phenol using the same method as above. The purity of the substance was 96 per cent. This study is also considered valid (Klimisch code 1).

Values of log K_{ow} were estimated for single components using the KowWin (v1.67) program within EPIWIN (v3.12) (USEPA, 2004) using the SMILES codes in Section 1.1.1. The results are presented in Table 1.3, along with available measured values.

Table 1.3 Predicted and measured log K_{ow} values.

	KOWWIN	Measured
Monostyrenated phenol	3.67	
2,4-Distyrenated phenol	5.83	6.24[a]
2,6- Distyrenated phenol	4.98	6.24[a]
Tristyrenated phenol	7.13	7.77

a – one measured value for both isomers.

The predicted values for the di- and tristyrenated components are lower than those measured. This suggests that the measured log K_{ow} for the monostyrenated component could be higher than the predicted value.

An alternative method to calculate log K_{ow} in the KowWin program uses a measured value for a related substance and calculates the value for the target substance based on the changes in structure. Using the measured values for di- and tristyrenated phenol, the log K_{ow} for monostyrenated phenol is calculated as 4.44 (three calculations using the two distyrenated isomers and the tristyrenated substance), which tends to suggest an underestimation in the original calculation. On the other hand, using measured values for phenol, *o*-cresol and *p*-cresol as the starting point gave a value of 3.58 which agrees well with the original prediction.

Predictions have also been obtained using the logP_Multicase program within the OECD (Q)SAR toolbox (OECD, 2008). For di-and tristyrenated phenol these are 7.03 and 9.63, which are much higher than the measured values.

The calculated value for monostyrenated phenol from KowWin was used in the assessment in the absence of other data, although on the basis of the above discussion there is some uncertainty in this value. The two measured values were used, as they were considered to be valid and suitable.

1.3.8 Hazardous physicochemical properties

Flash point

Flash point values above 180°C (open cup) and above160°C (closed cup) have been reported in IUCLID (2001) (Klimisch code 4).

1.3.9 Other relevant physicochemical properties

Viscosity

A value of 10,000 mPa.s is reported for the commercial product Wingstay F93 at 25°C (Tech Direct, 2005) (Klimisch code 4).

Henry's Law constant

A calculated Henry's Law constant value of 1.58×10^{-6} atm m^3/mol (0.16 Pa m^3/mol) has been reported for styrenated phenol (USEPA, 2003). This value was determined using the HENRYWIN (v3.10) program within EPIWIN (v3.12) (USEPA, 2004) at 25°C using a measured boiling point of 230°C.

Values of Henry's Law constant calculated at 25°C using EPIWIN v3.12 (HENRYWIN v3.10) for each component are given below. This program estimates Henry's Law constant from the chemical structure of the substances using the bond contribution method.

- Monostyrenated phenol 6.63×10^{-8} atm m^3/mol (6.72×10^{-3} Pa m^3/mol).
- 2,4-Distyrenated phenol 7.84×10^{-9} atm m^3/mol (7.94×10^{-4} Pa m^3/mol).
- 2,6-Distyrenated phenol 7.84×10^{-9} atm m^3/mol (7.94×10^{-4} Pa m^3/mol).
- Tristyrenated phenol 9.27×10^{-10} atm m^3/mol (9.39×10^{-5} Pa m^3/mol).

The following values of Henry's Law constant were determined using estimated values for water solubility and vapour pressure at 25°C using EPIWIN:

- Monostyrenated phenol 1.025×10^{-7} atm m^3/mol (1.04×10^{-2} Pa m^3/mol).
- 2,4-Distyrenated phenol 1.61×10^{-8} atm m^3/mol (1.63×10^{-3} Pa m^3/mol).
- 2,6-Distyrenated phenol 3.02×10^{-9} atm m^3/mol (3.06×10^{-4} Pa m^3/mol).
- Tristyrenated phenol 4.07×10^{-10} atm m^3/mol (4.12×10^{-5} Pa m^3/mol).

Henry's Law constant can be calculated for each component according to the approach set out in the Technical Guidance Document (EC, 2003):

Henry's Law constant = (vapour pressure (Pa) × molecular weight)/water solubility

The following Henry's Law constants were calculated according to the TGD method using the predicted vapour pressure values and the measured water solubility values:

- Monostyrenated phenol 5.6×10^{-3} Pa m^3/mol.
- 2,4-Distyrenated phenol 1.17×10^{-3} Pa m^3/mol.
- 2,6-Distyrenated phenol 1.17×10^{-3} Pa m^3/mol.
- Tristyrenated phenol 5.0×10^{-5} Pa m^3/mol.

As these values use measured water solubility data they are used in the assessment in preference to those calculated using predicted solubility values.

pKa

The pKa values for the three components have been calculated (SPARC Online Calculator available from: http://ibmlc2.chem.uga.edu/sparc/) as follows:

- Monostyrenated phenol 10.17.
- 2,4-Distyrenated phenol 11.20.
- 2,6-Distyrenated phenol 11.83.
- Tristyrenated phenol 11.99.

A composite pKa of 11.55 was selected for the distyrenated component.

These values mean that components will not be significantly ionised under environmental conditions.

Stability

The commercial product Westco SP-120 (CAS number 61788-44-1) is described as stable over a long period of time when stored in unopened containers and protected from extremes of temperature and humidity. It has a suggested shelf-life of two years (Westco, 2005).

1.3.10 Summary of physicochemical properties

A summary of physicochemical data used for the risk assessment is given in Table 1.4.

Table 1.4 Summary of physicochemical properties.

Property	**Monostyrenated phenol component**	**Distyrenated phenol component**	**Tristyrenated phenol component**
Molecular weight	198.27	302.42	406.57
Vapour pressure	6.53×10^{-3} Pa	2.57×10^{-6} Pa^{2}	8.69×10^{-10} Pa
Water solubility	**231 mg/l**	**0.665 mg/l**	**0.0071 mg/l**
n-Octanol-water partition coefficient (log K_{ow})	3.67	**6.24**	**7.77**
Henry's law constant[a]	5.6×10^{-3} Pa m^3/mol	1.17×10^{-3} Pa m^3/mol	5.0×10^{-5} Pa m^3/mol

Measured values are highlighted in bold. Unless stated otherwise, all calculated values given in this table were estimated using EPIWIN (v3.12).

[a] Values calculated in Section 1.3.9 from the measured solubilities and calculated vapour pressures.

2 General information on exposure

2.1 Production of styrenated phenol

2.1.1 Production processes

Industry information on the production of styrenated phenol is designated company-confidential (SPTF, 2005) and presented in the confidential annex to this report.

2.1.2 Production capacity

Data on production volumes are confidential, so are provided in the confidential annex to this report. Styrenated phenol (CAS number 61788-44-1) is listed as a high production volume chemical (HPVC) on the ESIS website. This substance is not classified. The following producers and importers of styrenated phenol are listed on the ESIS website. These data relate to the mid-1990s, and so do not relate to the present time.

Bayer AG
Cognis France
Degussa AG
Goodyear Chemicals Europe ECTC
Great Lakes Chemical Italia
Great Lakes Manufacturing GMBH
Huels AG
Lowi Polymer Stabilizers GMBH
Sidobre Sinnova

Tristyrylphenol (CAS number 18254-13-2) is listed as a low production volume chemical (LPVC) on the ESIS website, but is not classified in the Annex 1 of Directive 67/548/EEC. Rhodia Geronazzo S.P.A. is listed as a producer/importer of this substance.

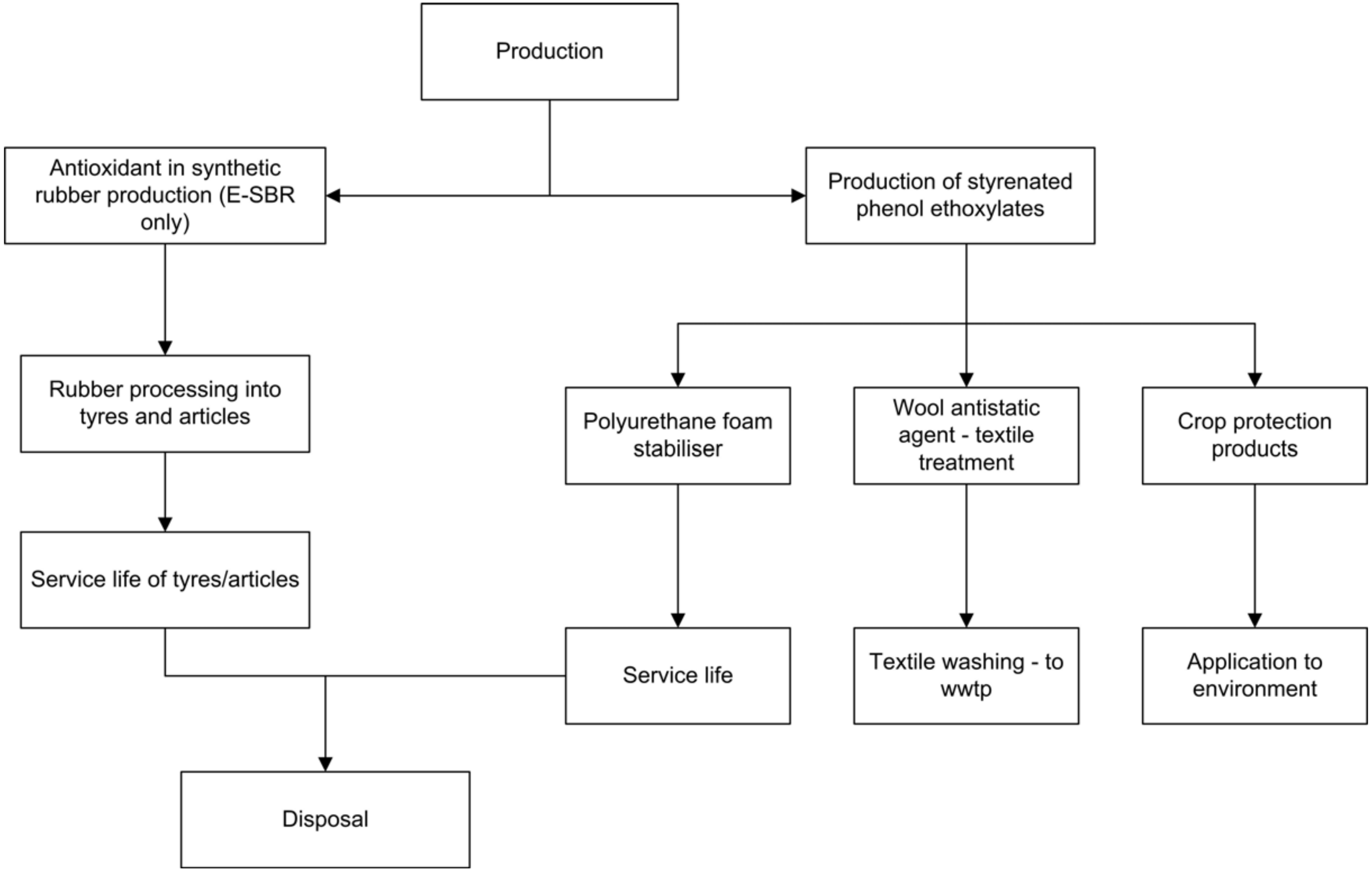
Information provided by industry confirms that styrenated phenol is produced and used in the EU. Consultation for this report identified four current producers in the EU – Cognis, Eliokem, Lanxess and Rhodia. The substance is not produced in the UK, but it is used in the UK. The life-cycle of styrenated phenol is illustrated in Figure 2.1.

2.2 Uses of styrenated phenol

2.2.1 General information on uses

Styrenated phenol is described as a non-staining, non-discolouring, non-migratory additive for natural rubber, synthetic rubber, adhesives, plastics, textile fibres, cable coatings, flooring, polyurethane foam, coated paper, and natural and synthetic oils (ACC, 2003; the Association of European Adhesives Manufacturers (FEICA), personal communication, 2006; Cognis, personal communication, 2005). The information gathered for this assessment identified the following two main areas of use in Europe.

Figure 2.1 Lifecycle of styrenated phenol in the EU.



Notes: possible emissions are considered from all points in the lifecycle shown in the figure. The crop protection products step is formulation of agrochemicals; any required formulation for polyurethane foam or textile treatment is included in the step shown.

- Antioxidant in rubber. The styrenated phenol blend used in this application is characterised by commercial product A (Section 1), with roughly equivalent levels of distyrenated and tristyrenated components.
- Intermediate in the production of primarily ethoxylated polymers (although other derivatives are produced) used mainly in crop protection products (Crop Protection Agency (CPA), personal communication, 2005). The styrenated phenol blend in this application is characterised by Commercial product B (Section 1), with the blend dominated by the tristyrenated phenol component. The crop protection product does not contain styrenated phenol in a non-ethoxylated (derivatised) form.

The possible use of styrenated phenol as an antioxidant in plastics has been mentioned. Consultation with potential user groups in the EU did not produce any evidence that such a use is made currently, although the responses covered only a small part of the potential users. In the absence of information that this use occurs, it was assumed for this assessment that all antioxidant use of styrenated phenol in the EU is in rubber. A summary of the uses of styrenated phenol, including whether the use is as an antioxidant or as a styrenated phenol ethoxylate, is given in Table 2.1. The table also indicates whether sufficient information is available on each use to take that aspect further in the assessment process.

Table 2.1 Uses of styrenated phenol.

General source application of styrenated phenol	Use	As styrenated phenol	As styrenated phenol ethoxylate[1]	Sufficient information for inclusion in this assessment
		Commercial product A	Commercial product B	
Antioxidant	Antioxidant in rubber (E-SBR)	yes		yes
	Antioxidant in plastic	Possible, no direct evidence		no
Intermediate in the production of surfactants	Surfactant in crop protection products		yes	yes
	Biocide in adhesives		unclear	no
	Textile fibres (as wool antistatic agent)		yes	yes
	Polyurethane foam stabiliser		yes	yes
Unknown source application (antioxidant or ethoxylate)	Paper coating	unknown	unknown	no
	Natural and synthetic oils	no	no	no

[1] Styrenated phenol is used as an intermediate in the formation of the ethoxylate.

At a late stage in the production of this assessment, information came to light about the use of styrenated phenol ethoxylates in emulsion polymerisation. The resulting emulsions are described as being used in industrial processes under strictly controlled conditions. It is not currently possible to assess this use further, although it appears unlikely to contribute significantly to the emissions (SPTF, 2009).

2.2.2 Use as an antioxidant in rubber

Antioxidants (stabilisers) are necessary additives to synthetic rubber to retard degradation. The mode of action of antioxidants such as styrenated phenol is a consequence of their role as hydrogen-donors. These inhibit the effects of oxidation by competing for peroxy radicals, with which they react to form hydroperoxides and prevent the abstraction of hydrogen from the polymer backbone (SpecialChem, 2005).

With styrenated phenol this produces a styryl phenoxy radical, which can combine with radicals formed in the rubber chain (and as a result is chemically bound into the rubber) or catalyse an elimination reaction in the rubber (which leads to regeneration of styrenated phenol). Other radicals can be formed from the styrenated phenol, and these can undergo similar reactions. The net effect is that over time the styrenated phenol becomes bound into the rubber and does not exist as a separate substance (SPTF, 2008a). This has implications when assessing the potential for leaching of styrenated phenol during the lifetime of the rubber product.

Antioxidants may be added at different stages in the production of rubber and rubber articles. Information from producers and users of styrenated phenol shows that this substance is added during the finishing step after polymerisation and before the coagulation step and storage (SPTF, 2005). Information provided by industry indicates that styrenated phenol is used exclusively as an antioxidant in the production of styrene-butadiene rubber by emulsion polymerisation (E-SBR) (Westco, 2005). Not all E-SBR produced in this way contains styrenated phenol; it is limited to non-oil extended forms.

A major use of rubber is in tyres. Information from tyre producers indicates that styrenated phenol is not added as an antioxidant during the production of tyres. However, E-SBR is used in the manufacture of tyres, and so styrenated phenol may be added through its presence in the E-SBR. It is estimated that 80 per cent of the E-SBR containing styrenated phenol is used in black rubber for tyres (Chemical Stakeholder Forum (CSF), 2005). For the manufacture of other rubber articles styrenated phenol is not thought to be added at this stage, but may be present through the use of E-SBR.

Data on production volumes for the use of styrenated phenol in the rubber industry are confidential and are presented in the confidential annex. These production figures and an assumed use level of 1 phr[7] are employed in the estimation of releases to the environment. A level of 1 phr has been described as a realistic maximum value for the use of styrenated phenol in E-SBR.

The life-cycle steps considered in the assessment for this area of use are:

- production of rubber;
- manufacture of rubber articles and tyres;
- service life of rubber articles and tyres;
- waste remaining in the environment from rubber articles and tyres.

More details on these steps are included in Section 3.

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[7] Parts per 100 parts of rubber by weight.

2.3 Intermediate for the production of surfactants

Styrenated phenol is used as a starting product in the production of emulsifiers and dispersing and wetting agents. These materials are produced through the modification of styrenated phenol through processes including ethoxylation (SPTF, 2006).

Because styrenated phenol is modified as part of the production of the surfactants it is presumed that the final product does not contain any styrenated phenol. This is confirmed for styrenated phenol used in the production of antistatic agents (in wool treatment) and stabilisers for polyurethane foams (Cognis, personal communication, 2005) and in crop protection products (Herdilla, 2005).

Information on the quantities of styrenated phenol used as intermediates in the production of surfactants is included in the confidential annex to this report. Data on emissions of styrenated phenol during the production of styrenated phenol ethoxylates for use primarily as agricultural agents are in the confidential annex (SPTF, 2007).

2.3.1 Crop protection products

Styrenated phenol is used as an intermediate for ethoxylated or propoxylated polymers which are used in the production of crop protection products (SPTF, 2005 and the European Council for Alkylphenols and Derivatives (CEPAD), no date). This is a key application for tristyrenated phenol (CEPAD, no date). Styrenated phenol is not present in the final product, only as the ethoxylate or propoxylated derivative (Herdilla, 2005).

The inclusion of styrenated phenol by the US Environmental Protection Agency (USEPA) in its list of pesticide ingredients as a List 3 chemical (inert ingredients of pesticides of unknown toxicity) (USEPA, 2006) is presumed to be a consequence of its use as an intermediate.

2.3.2 Biocide in adhesives

The identification of styrenated phenol as a biocide in adhesives was provided by the Association of European Adhesives Manufacturers (FEICA) (personal communication, 2006). No further information is currently available.

However, industry information suggests a preparation with antimicrobial properties can be produced by adding styrenated phenol and water to a heated mix of an alkyl phenol (unspecified) and a quaternary ammonium antimicrobial agent (SPTF, 2005).

Confirmation was sought as to whether it is the styrenated phenol or the preparation that has a biocidal effect. From the information available, it would appear that the styrenated phenol is not providing an antimicrobial function in the formulation. The inclusion of the styrenated phenol is probably as a surfactant. Styrenated phenol is not included in the listing produced under Commission Regulation (EC) 2032/2003 of the list of identified existing active substances and notified existing active substances. This supports the view that the styrenated phenol does not provide the antimicrobial function.

On the basis of the information received to date, it is concluded that the use of styrenated phenol in adhesives is restricted to their use as a surfactant precursor. However, as no specific quantities of styrenated phenol ethoxylate were identified for use in this application, this category was not considered further in this report, and an estimate of emissions from this application was not determined.

2.3.3 Wool fibre treatment

Styrenated phenol is used as an intermediate in the formation of a product used as an antistatic in wool fibre treatment (Cognis, personal communication, 2005). The final antistatic product does not contain styrenated phenol. Styrenated phenol itself is not an antistatic agent. Quantities of styrenated phenol used in the production of the antistatic product are presented in the confidential annex.

2.3.4 Foam stabiliser

Styrenated phenol, as the ethoxylate, is used as a stabiliser in polyurethane foam (Lanxess, personal communication, no date). Information on the quantity of styrenated phenol used in this application is presented in the confidential annex.

2.3.5 Degradation of styrenated phenol ethoxylates

The assessment of other phenol ethoxylates, such as those produced using nonylphenol, has shown that degradation of the ethoxylate during the use and disposal phases of its lifecycle results in the release of the phenol component (for example nonylphenol) into the environment.

A similar situation is expected to occur with styrenated phenol ethoxylates. These emissions are considered in Section 3.

2.3.6 Summary for ethoxylate uses

The following life-cycle steps relating to the use of styrenated phenol are considered in this assessment.

- production of styrenated phenol ethoxylates;
- formulation of products containing styrenated phenol ethoxylates;
- use of agrochemicals containing styrenated phenol ethoxylates (releases as ethoxylates);
- treatment of wool as anti-static agents including releases on subsequent washing of treated wool in garments;
- use as stabilisers for polyurethane foams.

For all but the first of these life-cycle steps, emissions are estimated as amounts of ethoxylates which are then converted to amounts of styrenated phenol (Section 3.1.3).

2.4 Other uses

In addition to the uses already described, the American Chemistry Council lists paper coatings and natural and synthetic oil applications for styrenated phenol (ACC, 2003).

2.4.1 Paper coatings

Information from the Paper Chemicals Association (PCA) report indicates that styrenated phenol is included in the current Draft 19 of the Council of Europe (CoE) list of substances deemed acceptable for use in paper and board for food packaging (PCA, no date). This suggests that styrenated phenol is, has been, or is proposed to be used in one or more paper processing chemicals (PCA, no date). However, the PCA add they have no records of such a use. Information from the company that responded to a request for information in this area supported this conclusion.

Further information, including a basic description of the general use of styrenated phenol in paper coatings, was not found. Styrenated phenol type compounds are also not described in the Emission Scenario Document on Pulp, Paper and Board Industry (Environment Agency, 2007a).

On the basis of discussions with the Paper Chemicals Association and the absence of the listing of styrenated phenol in the Emission Scenario Document (ESD) on Pulp, Paper and Board Industry, the use of styrenated phenol in paper coatings was not considered further in this assessment.

2.4.2 Natural and synthetic oils

Although further information was sought to clarify usage in this area, no information was identified[8]. In the absence of further information the potential application of styrenated phenol in natural and synthetic oils was not considered further.

2.5 Production and use volumes

Information was provided by industry on EU market volumes for styrenated phenol (SPTF, 2005). This is presented in the confidential annex.

2.6 Trends

The styrenated phenol market is considered mature and no major developments in usage are expected. Use of styrenated phenol as a raw material in the production of surfactants for use in crop protection products has increased since 2003 due its use as a replacement for ethoxylated nonylphenol surfactants. Industry expects few developments in this area in Europe in the next few years (SPTF, 2005).

2.7 Regulatory initiatives

Styrenated phenol is included in the list of chemicals of concern of the UK Chemicals Stakeholder Forum. It was assessed as a potential PBT/vPvB substance by the EU PBT Working Group and further testing was required under Commission Regulation (EC) No 465/2008.

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[8] Only one reference to a styrenated phenol based lubricant was identified. This is the Montaclere SPH reported to be produced by Flexsys. However, this compound, or other styrenated phenol-based lubricants are no longer produced by Flexsys.

Styrenated phenol is included in the US Environmental Protection Agency High Production Volume Challenge Program, in the styrenated phenols category.

3 Environmental exposure

3.1 Environmental releases

3.1.1 General introduction

The purpose of this section is to review releases of styrenated phenol to the environment. The composition of the commercial product varies according to the intended use and the physicochemical characteristics are different for each of the three components. Consequently, estimation of the environmental releases of this substance is complex. To reflect these differences, this assessment was conducted separately for the three components: monostyrenated phenol, distyrenated phenol and tristyrenated phenol. Two commercial products representative of use types and specific quantities of mono-, di- and tristyrenated phenols were used in the assessment. These are:

- Commercial product A (representative of the styrenated phenol used as an antioxidant in rubber):
  - Monostyrenated phenol 11 per cent.
  - Distyrenated phenol 43 per cent.
  - Tristyrenated phenol 43 per cent.
- Commercial product B (representative of the styrenated phenol used in the production of styrenated phenol ethoxylates):
  - Monostyrenated phenol 2 per cent.
  - Distyrenated phenol 23 per cent.
  - Tristyrenated phenol 70 per cent.

For example, a release of 10 kg of styrenated phenol as commercial product A is assumed to contain 1.1 kg monostyrenated phenol, 4.3 kg distyrenated phenol and 4.3 kg tristyrenated phenol. Although this approach makes a number of assumptions (such as, all commercial forms of styrenated phenol used as an antioxidant in rubber have the same composition of mono-, di-, and tristyrenated components), it is considered representative and appropriate for addressing environmental risks from styrenated phenol.

The background to the scenarios considered in the assessment is explained fully in the Technical Guidance Document (EC, 2003). The 'local environment' represents the environment near a site of release (for example a production, formulation or processing site). Emissions for estimating local concentrations are calculated on a kg/day basis for realistic worst case situations, for example for larger sites operating a process. The 'regional environment' represents a highly industrialised area 200 km × 200 km with 20 million inhabitants, and it is assumed that 10 per cent of the total EU production and use takes place in this area (exceptions to this are noted in the text). The 'continental environment' is the remainder of the EU and represents "background" concentrations. Emissions for these two larger scales are estimated on an annual basis.

The following sections describe modelled releases to the environment, estimated using data from various sources. Industry-specific information was used in preference where available; in the absence of this, emission scenarios were used and finally the default emission factors given in Appendix I of the TGD. Industry-specific information is limited and therefore much of the information used is generic in nature and not necessarily specific to styrenated phenol.

A note on the use of emission factors in this assessment. Emission scenario documents provide emission factors to apply to the amount of a substance used in a process to estimate the emission. In many cases these factors do not depend on the properties of the substance, and so the same emission would be calculated for substances with different properties. In the case of styrenated phenol, this means that the three components are assumed to be lost in the same ratio that they are present in the commercial product (or the emission is calculated as styrenated phenol, and then divided into the three components in the composition ratio). This is a simplification, but in the absence of other information has been applied here. In some cases, such as the production of rubber and service life of rubber articles, the properties of the substances can be taken into account to some extent, and so for these individual releases are calculated for each component. These cases are identified in the text.

The calculations use information provided on the quantities used in each area. This information is confidential as only a small number of producers are involved. Where possible, release estimates have been included in this document (where the amount used at a site is generic information, for example). For regional and continental releases in particular, the emission estimates would allow the amounts to be determined, and so they are included in the confidential annex.

3.1.2 Releases from the production of styrenated phenol

Production losses

Information was provided on the emission control and waste management measures in place at the major production sites. Most of this is confidential and is included in the confidential annex. The nature of the production process means that no water is involved. This information is considered to be relevant to the smaller production sites as well. On the basis of this information, the emissions from this life-cycle step were considered to be negligible, and were not considered further in this assessment.

Transportation losses

Chemicals can be released to the environment during loading of transport containers at production sites and unloading containers at the sites where the substance is used. These losses can take the form of spillages (to wastewater) or volatilisation. As styrenated phenol has a low vapour pressure at room temperature, any volatile losses to the atmosphere from loading or emptying containers are considered negligible. Because styrenated phenol is transported in liquid form, no emissions as dust are likely to occur (Cognis, personal communication, 2005).

3.1.3 Releases from use as an antioxidant in rubber

Releases from production of rubber

As noted in Section 2.2.2, antioxidants are added to the rubber emulsion after the polymerisation process has been stopped. The default emission factor from the TGD for a stabiliser used in a wet polymerisation process is 0.05 per cent, but the addition of the styrenated phenol follows the polymerisation process so this may not be the most appropriate value. The emulsion to which the styrenated phenol is added consists of an organic phase dispersed in water, with various agents to produce and maintain the emulsion. The subsequent processing of this material to give the rubber crumb involves breaking the emulsion and washing the product. The styrenated phenol will partition between the aqueous and organic phases, with a preference for the organic phase especially for the di- and tristyrenated components.

Eliokem (2007) carried out laboratory scale studies on the content of styrenated phenol in the wastewater from the coagulation of latex to which the substance had been added following polymerisation. Water was sampled from the initial coagulation step and from two subsequent washing steps. None of the three components was detected in any of the water samples, at a detection limit of 80 µg/l for each component. Both mono- and distyrenated phenols have measured solubilities above this level, and so could have been detected had they been present at close to solubility.

Some indication of the level of styrenated phenol in water can be obtained by assuming that the octanol-water partition coefficient can be used to estimate partitioning between the water and organic (rubber) phases. It is also assumed that the concentration of styrenated phenol in the rubber phase is that intended to be reached, that is one per cent as the total of the components. Some of the organic phase may be left in the aqueous phase on separation. Against this, styrenated phenol should have a strong affinity for the rubber on the basis of similar structures, more so than for octanol, and hence the log K_{ow} probably underpredicts the rubber-water partition. Overall, the approach taken should not underestimate the amount lost in water.

The predicted log K_{ow} value for monostyrenated phenol is 3.67. This component makes up 11 per cent of the added material, so the concentration in rubber is 1.1 g/kg. Considering rubber and octanol to have similar partitioning properties for this calculation, this concentration in rubber would be in equilibrium with a concentration of 0.24 mg/l in water to give the log K_{ow} value. This would have been detectable at the given detection limit, and is below the solubility. It is possible that the styrenated phenol component partitions more to the rubber phase than is estimated by the log K_{ow} value or that the K_{ow} is an underestimate (see Section 1.3.7). The measured log K_{ow} for the distyrenated component is 6.24, which is somewhat higher than the calculated values of 4.98 and 5.83. A log K_{ow} of 4.1 would give a water concentration of around 80 µg/l for the monostyrenated component. As a worst case, it is assumed that the concentration of monostyrenated phenol in the wastewater is 80 µg/l.

For the distyrenated component, the concentration in the rubber is 4.3 g/kg; with a measured log K_{ow} of 6.24, this gives a concentration in water of 2.5 µg/l. This would not have been detected, and so does not contradict the observed results. A similar calculation for the tristyrenated component gives a water concentration of 0.07 µg/l. In both cases the estimated concentration is below the measured solubility. For the purpose of estimating emissions from this process, the concentrations calculated here are assumed.

Information provided by industry (SPTF, 2007) provides a figure of 21 litres of water used per kilogram of rubber. Using this volume with the concentrations estimated above gives the following emission factors:

Monostyrenated – 1.7 mg/kg rubber

Distyrenated – 53 µg/kg rubber

Tristyrenated – 1.4 µg/kg rubber

These are applied to generate emissions of each component; a composite estimate is not made.

The largest site producing E-SBR in the EU produces 120,000 tonnes of rubber per year (BREF, 2007). For production over 300 days, this is 400 tonnes per day. It is assumed for the purposes of the local emission estimates that all of the rubber produced on the day contains styrenated phenol as the antioxidant. From the emission factors above, emissions of the three components to wastewater are:

Monostyrenated – 0.68 kg/day

Distyrenated – 0.021 kg/day

Tristyrenated – 0.59 g/day

For the annual emissions, it is assumed that the site will produce rubber containing other antioxidants. For the EU, 70 per cent of the E-SBR produced is of the non-oil extended form in which styrenated phenol can be used (see Section 2.2.2). As other antioxidants can be used, it is assumed that styrenated phenol accounts for 33 per cent of the antioxidant used in this type of rubber. Hence the annual production at this site of rubber containing styrenated phenol is 27,720 tonnes, and the annual emissions are:

Monostyrenated – 47 kg/year[9]

Distyrenated – 1.5 kg/year

Tristyrenated – 0.04 kg/year

These emissions are used as the regional emissions, as the site uses more than 10 per cent of the amount used for this purpose. The continental emissions were estimated in the same way, and are included in the confidential annex.

Release from production of tyres

Information from the rubber industry indicates that styrenated phenol is not added during the processing of rubber in the production of tyres. However, E-SBR is used in the production of tyres, and so styrenated phenol may be already present in the rubber used. The following calculations are based on this.

OECD (2004b) provides information on the rubber industry, and this was used in the absence of more specific information. A representative site is considered suggested to produce 33 tonnes of tyres per day. The E-SBR containing styrenated phenol is only used in the tread, which makes up 30 per cent of the weight of the rubber in the tyre (SPTF, 2008b). Hence the relevant amount of rubber is 9.9 tonnes per day.

Kirk-Othmer (2004) provides typical compositions of tyre tread material. For standard tyres this is:

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[9] Example: 27,720 tonnes/year × 1.7 mg/kg released → 47 kg/year for monostyrenated.

SBR	50-100 phr
BR	0-50 phr
Carbon black	70-80 phr
Oil	30-60 phr
Others	7-10 phr

Taking the middle of the range values for each component, SBR makes up about 33 per cent of the total. Information provided by industry (SPTF, 2008b) indicates that only 70 per cent of this SBR will be non-staining E-SBR. Hence, the amount of rubber containing styrenated phenol is 9.9 × 33 per cent × 70 per cent or 2.3 tonnes per day[10].

From OECD (2004b) local emissions to wastewater are calculated with the equation:

$$E_{local} = Q_{prod} \times \frac{Q_{add}}{100 \bullet F_{recipe}} \times \left(1 - F_{rem}\right)$$

Where Q_{prod} is the amount of rubber containing styrenated phenol used (2.3 tonnes/day)

Q_{add} is the level of use of the additive (one per cent)

F_{recipe} is 1 when the level is expressed as a percentage by weight

F_{rem} is the fraction of the additive remaining in the product

The suggested default value for F_{rem} for antioxidants in tyres is 0.99. The properties of styrenated phenol suggest that it will be retained to a greater extent than this. Laboratory tests on the amount of styrenated phenol found in water following E-SBR production (Eliokem, 2007, see *Releases from production of rubber* above) showed no detection of styrenated phenol at 80 µg/l. These results were converted above into an emission of 1.75 mg/kg rubber (as the sum of the three components); at a level of one per cent in rubber, this is an emission of around 0.02 per cent to water (based on the detection limit). This corresponds to a F_{rem} value of 0.9998. Taking the log K_{ow} value for monostyrenated phenol (3.67), the concentration ratio between octanol and water is approximately 5,000:1. The nature of styrenated phenol and its similarity to the structure of the rubber suggests it would be more compatible with rubber than with octanol. The log K_{ow} for the di- and tristyrenated components are higher, so they would be expected to be retained to a greater extent. This and the fact that the value of F_{rem} of 0.9998 is based on the detection limit means this a conservative approach.

The calculated emission is 4.6×10^{-3} kg/day. This is divided between the three components in the ratio of the composition of Product A, giving emissions of 5.06×10^{-4} kg/day for monostyrenated phenol, and 1.98×10^{-3} kg/day for both di- and tristyrenated phenol.

The regional and continental release estimates are confidential, and are included in the confidential annex, but are calculated by applying the ($1-F_{rem}$) value to the regional and continental tonnages. From information provided to the Chemical Stakeholder Forum (CSF, 2005), an estimated 80 per cent of the E-SBR containing styrenated phenol is

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[10] Other antioxidants can be used in non-staining E-SBR (styrenated phenol accounts for 30 per cent of the production), but information from industry (SPTF, 2008b) indicates that non-staining E-SBRs with different antioxidants would not be mixed in the same tyre. Hence, it is assumed for the local calculations that all of a day's production uses non-staining E-SBR containing styrenated phenol.

used in black rubber for tyres, and so these calculations are applied to 80 per cent of the total used as an antioxidant in rubber.

Release from production of other rubber articles

The same approach is adopted as for tyres. It is assumed that styrenated phenol is present in E-SBR used in the production of articles. The European Tyre and Rubber Manufacturers Association (ETRMA, 2008) have confirmed that styrenated phenol is not added as an antioxidant at this stage, and is only present as a result of use during the production of E-SBR.

From OECD (2004c) the amount of rubber used at a representative site for other articles is 22 tonnes per day. The ESD divides this between a range of product types. Industry (SPTF, 2008b) considered it reasonable to assume a site would produce only one or a limited range of products, at least at one time, and that all of the production could involve the use of E-SBR. Hence the total daily production of 22 tonnes is used as the basis for these estimates.

Information from industry (SPTF, 2008b) indicates that the composition of the rubber used is likely to be similar to that in tyres. Assuming 33 per cent of the rubber is SBR, of which 70 per cent is non-staining E-SBR, gives the relevant amount of rubber (Q_{prod}) as 5.1 tonnes per day. As for tyres, it is assumed that different types of non-staining E-SBR (containing different antioxidants) are not mixed in the same article. Use of styrenated phenol is taken as one per cent, and the fraction remaining (F_{rem}) as 0.9998 as derived above. From these values E_{local} is calculated as 0.01 kg/day. This is divided between the three components as for tyres, giving emissions of 1.1×10^{-3} kg/day for monostyrenated phenol, and 4.3×10^{-3} kg/d for both di- and tristyrenated phenol.

The regional and continental release estimates are calculated as for tyres, applying the ($1-F_{rem}$) factor to 20 per cent of the total tonnage for antioxidant use in rubber. The results are in the confidential annex.

Release from the use of tyres

This section uses the same approach as employed in the risk evaluation for 4-*tert*-octylphenol (Environment Agency, 2005b). Losses from tyres in use are possible, through abrasive wear of the material rather than through leaching or volatilisation. Information from Australia suggests that an average new tyre weighs 10 kg and a used tyre weighs about 9 kg. The weight of rubber (polymer and all additives) is 85 per cent of the total tyre weight, so about 12 per cent of the rubber is lost during the service life of the tyre (SA EPA, 2002). An Environment Agency report (Environment Agency, 1998) suggests losses of 10-20 per cent of tyres by weight over their lifetime, with a total loss in the UK of 53,000 tonnes of rubber per year. This total corresponds to 14 per cent of the weight of tyres disposed of each year. An average of 15 per cent is used to estimate losses of rubber per year. Assuming that the new rubber processed into tyres goes to replace that withdrawn from use at the end of the tyre service life, the equivalent of 15 per cent of new rubber will be released each year.

Styrenated phenol is intended to react with active species to protect the rubber, and so is degraded in use. It is estimated that about 20 per cent of the substance remains at the end of the useful life of products[11]. The average content over the lifetime is taken

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[11] Based on analytical results for the fate of amine antioxidant compounds (6PPD and DPPD/DTPD) from new and aged tyres, which showed that at least 85 percent of the additives were degraded over the product lifetime (Umweltbundesant (UBA), 1997). A value of 80 per cent is used here as a conservative estimate for a different type of antioxidant.

as 60 per cent ([100+20]/2). This release is assumed to be split equally between surface water and industrial soil (for example, roadside verges), with 10 per cent release to the region. Not all of the styrenated phenol present in the abraded material might be available to the environment, but for the purpose of this assessment complete availability is assumed in the absence of more information. It is also possible that further reaction of the styrenated phenol could take place in the particulate material before release can take place, so this assumption will tend to overestimate emissions.

The actual emission values are included in the confidential annex.

Release from the use of rubber articles

Losses may occur from other rubber articles in use. There is no information available for styrenated phenol. The approach used in the emission scenario document for plastics additives (OECD, 2004b) is used here. This approach estimates emission factors to air and water based on a comparison of the properties of the substance being assessed with those of a model substance, diethylhexylphthalate (DEHP). Substances are considered as high, medium and low volatility or solubility. Note that these terms are in relation to DEHP and not as would be used generally.

For emissions to air, DEHP is considered to be a medium volatility substance, and an emission factor of 0.05 per cent over the lifetime is used. DEHP has a vapour pressure of 2.2×10^{-5} Pa. In comparison, monostyrenated phenol has an estimated vapour pressure of 6.5×10^{-3} Pa and is considered of high volatility; hence an emission factor of 0.25 per cent over the lifetime is used. Distyrenated phenol has an estimated vapour pressure of 2.6×10^{-6} Pa, and is considered of low volatility; an emission factor of 0.01 per cent is used. The vapour pressure of tristyrenated phenol is estimated to be very low, so that volatile emissions are considered to be negligible.

The solubility of DEHP is 3 µg/l, which is considered low. Monostyrenated phenol has a solubility of 231 mg/l, which is taken as highly soluble. Distyrenated phenol has a solubility of 0.66 mg/l, which is considered as medium solubility. Tristyrenated phenol has a solubility below 25 µg/l and is considered as low solubility.

Emissions to water are considered for indoor and outdoor situations. There is no information on the actual division of use for rubber articles containing styrenated phenol, so an even split (50:50) is used. The indoor emission factor for DEHP is 0.05 per cent. Based on the comparison above, the factors for mono-, di- and tristyrenated phenol are 0.5, 0.25 and 0.05 per cent respectively. These are over the service life.

The outdoor emission factor for DEHP is 0.15 per cent per year. Again, based on the comparison above, the factors for mono-, di- and tristyrenated phenol are 1.5, 0.75 and 0.15 per cent per year, respectively. An average service life value of 10 years is assumed, leading to overall emission factors for mono-, di- and tristyrenated phenol of 14, 7.25 and 1.5 per cent over the service life respectively (the values are adjusted for the reduction in the amount available for release from one year to the next).

The composition of styrenated phenol in the rubber is taken as that in the substance as added, commercial product A. As with the use in tyres, styrenated phenol will be degraded in use, and the same assumption of 20 per cent left at the end of the service life is used, so that the average concentration is 60 per cent of that added. Releases are calculated by applying the emission factors to the initial amounts, and then reducing the resulting values to 60 per cent.

The resulting total emissions are summarised in Table 3.1. The regional emissions are taken as 10 per cent of the totals; the continental emissions are the other 90 per cent.

Indoor emissions to water are considered to go to wastewater, outdoor emissions to water go directly to surface water.

Table 3.1 Service life emissions from rubber articles.

Substance	Air (kg/year)	Indoor water (kg/year)	Outdoor water (kg/year)
Monostyrenated phenol	30	30	832
Distyrenated phenol	4.6	58	1,683
Tristyrenated phenol	-	12	348

Release from waste remaining in the environment

The final losses to be considered are losses associated with waste in the environment. Losses of particulates to the environment can occur through wear and abrasion. They fall into two categories, particulate waste generated during the service life of the products, and losses on disposal. The losses of particulates from tyres have already been addressed in the section on tyre service life above. The risk evaluation for 4-*tert*-octylphenol (Environment Agency, 2005b) concludes that releases from the disposal, re-use or use in other areas of tyres make a negligible contribution to the overall emissions. The same can be applied to styrenated phenol (the vapour pressure of all three components is lower than that of octylphenol, and the solubilities of the two main components are lower, hence emission by volatilisation and leaching will be lower). Therefore this section only considers waste in the environment for other rubber articles.

No agreed method is currently included in the TGD for addressing these potential sources of release. These emissions were considered in the draft EU risk assessments of several phthalate plasticisers and flame retardants (for example, decabromodiphenyl ether, ECB, 2000). A similar approach is taken here. Service life factors are applied to the annual tonnage of the substance used in the individual areas. Disposal factors are applied to the amount of substance remaining at the end of the service life, taking into account losses estimated at formulation, processing, and over service life (both substance losses and particulate losses as estimated using the factors in this section). As the service life emissions have been calculated for each component, the waste in the environment calculations are also for each component.

As there is no information on the nature of products containing E-SBR with styrenated phenol, a generic release factor of two per cent of the rubber (and hence the substance) is used for both of these steps for rubber articles. The distribution of these emissions between environmental compartments follows that in other ESR assessments, and is 75 per cent to urban soil, 24.9 per cent to surface water and 0.1 per cent to air.

The resulting emissions are in Table 3.2. For the purpose of this assessment it is assumed that the substance in particulate emissions is available to the environment; as noted in the section on particulates from tyres, this is likely to be an overestimate.

Table 3.2 Emissions from rubber articles as waste in the environment.

	Regional (kg/year)			Continental (kg/year)		
	Air	Surface water	Industrial soil	Air	Surface water	Industrial soil
Monostyrenated phenol	0.03	7.8	23	0.3	70	210
Distyrenated phenol	0.12	31	92	1.1	275	827
Tristyrenated phenol	0.12	31	92	1.1	276	831

Ultimate disposal

Disposal by landfill or incineration is likely to be the ultimate destination for many of the products containing antioxidants. It is likely that some styrenated phenol may remain present in articles at disposal.

OECD (2004b) considers incineration likely to completely destroy antioxidants.

In landfills, any remaining antioxidant may be subject to leaching, volatilisation and degradation. It is currently not possible to quantify releases from landfills. However, styrenated phenol is expected to adsorb strongly onto soil and so leaching and volatilisation from landfill would not be expected to be significant processes compared with other sources of release.

3.1.4 Releases from the production and use of surfactants

A key area of use of styrenated phenol is as an intermediate in the production of surfactants. These surfactants are used primarily by the agrochemical industry in crop protection products, but also have minor applications as wool antistatic agents and foam stabilisers. Information on the quantity of styrenated phenol used for these applications is presented in the confidential annex to this report.

Surfactants can be produced from styrenated phenol using a number of different reactions, including ethoxylation and propoxylation. For simplicity, these are all referred to as ethoxylates in this assessment. Information provided by industry indicates that for a typical product one kg of styrenated phenol produces 3.9 kg of ethoxylate, and this conversion is used where necessary[12]. The composition of the styrenated phenol used in this area is that of commercial product B.

Releases are estimated in the following sections from the production of surfactants and from the subsequent formulation and use of these products. With the exception of the surfactant production stage, the emissions are of the ethoxylate. These are subsequently converted to styrenated phenol as indicated in the text.

In some places in this assessment, the vapour pressure of ethoxylates is referred to, or is used in estimating emissions. No actual data on these substances were identified for this assessment; instead values were calculated using EPIWIN (USEPA, 2004) for a representative structure, tristyrenated phenol with 28 ethoxylate units. The resulting value is zero, so the vapour pressure is taken to be negligible. Although this value has considerable uncertainty, it is only used to give an indication of the likely behaviour of the ethoxylate substances.

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[12] This corresponds to a tristyrenated substance with approximately 28 ethoxylate units.

Releases from surfactant production

Information provided by the major producer of surfactants from styrenated phenol indicates that there are no significant emissions from that site. No similar information is available for other companies producing surfactants using styrenated phenol, and so the default values from the TGD are used. The default emission factor for use as an intermediate is 0.7 per cent (Table A3.3 in the TGD). Note that this is the factor for a high tonnage substance, as the overall tonnage is greater than the relevant threshold. Using the total quantity used for this purpose, Table B3.2 in the TGD gives the number of days used as 141. Information was provided on the likely size of a representative company using styrenated phenol for this purpose, and this was used to estimate local emissions. These are confidential, and are included in the confidential annex. The emission factor does not depend on the properties of the substance, so the emissions of each component are assumed to be in the same ratio as the substance used (product B).

Regional and continental emissions were also estimated. These take account of the fact that the largest user does not have significant emissions. These estimates are in the confidential annex.

Releases from the formulation of products containing styrenated phenol ethoxylates

Information on the formulation of styrenated phenol derivatives (including styrenated phenol ethoxylates) for use as surfactants in the EU wasprovided by industry and is included in the confidential annex to this report. This relates mainly to the formulation of agrochemical products.

The largest site identified is used as the basis for local emission estimates as a worst case situation. Emissions here are of the ethoxylate at this stage. The default emission factors for formulation (Table A2.1 in the TGD) are 0.3 per cent to wastewater, and 0.25 per cent to air. However, the negligible predicted vapour pressure of the ethoxylates indicates that volatile emissions are unlikely, and so this route is not be considered in the calculations. Operation is over 300 days. The estimated emission to wastewater is confidential, and is included in the confidential annex.

Information from a small number of formulators indicates that at these sites, washings and/or waste materials are incinerated with no releases to the environment. As these formulators constitute only a small fraction of the number of users, the default emission estimates were retained. However, individual sites may have much lower or negligible emissions. In many cases, the nature of the products being formulated (products containing active agents) should mean that emissions are strictly controlled.

This scenario is considered to cover all of the formulation operations using styrenated phenol ethoxylates. It is not clear whether there is a formulation step for the use of the ethoxylates in stabilisation of polyurethane foams, as it is possible to add substances at the point of mixing the main components to produce the foam.

The site used in the calculations above accounts for more than 10 per cent of the amount used in this area, and so is used for the regional emissions as well. These and the continental emissions are included in the confidential annex.

Releases from the use of agrochemical formulations containing styrenated phenol ethoxylates

This is the major use of the styrenated phenol ethoxylates. It is assumed that in use, all of the ethoxylate in the formulation will be released to the environment. The Pesticides Safety Directorate (PSD, 2008) provided information on the standard scenario used in assessing crop protection products. For this, it is assumed that the equivalent of 2.77 per cent of the application rate drifts onto water, and this is used in the calculation of local concentrations in water (Section 3.3.1). Application at a typical rate is assumed in the calculation of concentrations in soil (Section 3.3.2). For the regional and continental emissions it is assumed for this assessment that 2.77 per cent of the amount used is released to water, and the rest to soil. The estimated releases on the regional and continental scales are included in the confidential annex.

Note that these are releases of ethoxylates; these are converted to releases of styrenated phenol later.

Use of styrenated phenol ethoxylates as wool antistatic agents

No information on releases from this use area was located. The following estimates are based on information in the Emission Scenario Document on Textiles (OECD, 2004a). Treatment with an anti-static agent is considered as functional finishing. The default size of textile plant in the ESD produces 13 tonnes of textile per day ($Q_{textile}$), operating on 225 days per year. It is assumed that not all of one day's production will be treated with the same substances, and a value of 30 per cent is proposed for the fraction treated with an individual substance ($F_{product}$). The ESD has a use rate of two per cent (20 kg/tonne) for the amount of substance used ($Q_{product}$ for textile auxiliaries, in padding liquors for functional finishing). The content of the styrenated phenol ethoxylate in the preparation used is taken as one, the default for $S_{ubstance}$. The degree of fixation of the substance to the textile ($F_{fixation}$) is taken to be 100 per cent, but there will be some substance in the spent padding bath liquors, and a value of 10 per cent is proposed for this ($F_{residual\_liquor}$).

The estimated emissions are therefore:

$$
\begin{aligned}
Elocal_{water} = \quad & \{Q_{textile} \times F_{product} \times Q_{product} \times C_{substane} \times (1 - F_{fixation})\} + \\
& \{Q_{textile} \times F_{product} \times Q_{product} \times C_{substane} \times F_{residual\_liquor}\} \\
= \quad & (13 \text{ tonne/day} \times 0.3 \times 20 \text{ kg/tonne} \times 1 \times (1-1)) + \\
& (13 \text{ tonne/day} \times 0.3 \times 20 \text{ kg/tonne} \times 1 \times 0.1) \\
= \quad & 7.8 \text{ kg/day to wastewater}
\end{aligned}
$$

The site used for the calculations accounts for more than 10 per cent of the total EU usage, and so the regional emissions are based on this site. The regional and continental emissions are in the confidential annex.

Kirk-Othmer (2000) includes nonylphenol ethoxylates among the non-durable anti-static agents, which are those which will be removed on washing. It is assumed that styrenated phenol ethoxylates will also be removed through washing, and that they will pass to a wastewater treatment plant. It is also assumed that the amount washed off per year is equal to the amount used per year, less the emissions at the application stage. The regional release is taken as 10 per cent of the total. These values are included in the confidential annex.

Polyurethane foam stabilisers

No information on releases of styrenated phenol ethoxylates from this use was located. The following discussion is based on treatment of losses from the production of polyurethane foams in the risk assessment for tris(2-chloro-1-methylethyl) phosphate (TCPP) (Environment Agency, 2007b). TCPP is used as a flame retardant in polyurethane foams.

The TCPP risk assessment concludes that losses from the foaming process are essentially zero. The foaming process is enclosed, and fumes are extracted through an activated carbon filter or through other abatement methods, and the volatile losses of TCPP are considered to be negligible. TCPP has a vapour pressure of 1.4×10^{-3} Pa; the vapour pressure calculated for a 28-ethoxylate unit styrenated phenol ethoxylate is negligible (see Appendix 2, Section A2.4) and so emissions of the ethoxylate are also considered negligible. The foaming equipment is not cleaned with water but with solvent which is collected and sent for treatment, hence there are no emissions to water. There will be loss in waste product, which will go to landfill (the estimate is 0.2 per cent, this is not considered further here).

There may be volatile emissions during the curing and storage of the foam. These are estimated as 1.2×10^{-4} per cent for TCPP. Considering the relative vapour pressure of the ethoxylate compared to that for TCPP, the volatile emissions can be considered to be negligible. There are no losses to water from this step.

In service, again losses to air are possible. A factor of 9.6×10^{-3} per cent is estimated for TCPP in the assessment; as the volatility of the ethoxylates is so much lower, any volatile losses can be neglected. Polyurethane foams are rarely used in situations where they come into contact with water, and so leaching losses are also negligible.

Hence, there are no major releases from the use of ethoxylates in polyurethane foams.

Releases of styrenated phenol from the degradation of surfactants

The risk assessment conducted for nonylphenol (European Chemicals Bureau (ECB), 2000) identified the potential for ethoxylates (produced using nonylphenol as an intermediate) to degrade in wastewater treatment plants and the environment to nonylphenol. A similar approach was used here to estimate the potential release of styrenated phenol from the degradation of ethoxylates. The fractions used were adjusted to take account of the different composition of the styrenated phenol ethoxylates compared to those produced from nonylphenol. No data were located on the degradation of styrenated phenol ethoxylates themselves, and so these calculations are based on data for octyl- and nonylphenol ethoxylates.

For nonylphenol, degradation in the wastewater treatment plant (mainly during anaerobic digestion of sludge) was estimated to lead to the release of nonylphenol to surface water equivalent to 2.5 per cent of the weight of ethoxylate entering the plant. Similarly, 19.5 per cent of the weight of ethoxylate entering the plant was estimated to be found in sludge as nonylphenol. Nonylphenol typically makes up 40 per cent by weight of the ethoxylates (the rest being ethoxy units), and so the overall “yield” of nonylphenol is 55 per cent of the amount used to make the ethoxylates.

The extent of degradation of ethoxylates is considered likely to be similar for styrenated phenol. It is similar for nonyl- and octylphenol, although as these have similar structures this is not clear evidence, but it suggests that ethoxylate chains have a similar susceptibility to degradation. Therefore, the same yield of 55 per cent is applied to the degradation of styrenated phenol ethoxylates in treatment plants. This gives the amount of styrenated phenol released to water as 1.56 per cent and the amount to sludge as 12.7 per cent, based on the amount of ethoxylate entering the plant. These estimates have a degree of uncertainty, as there are no data for styrenated phenol ethoxylates to support them.

For releases to surface water and to soil, the nonylphenol assessment uses a value of 2.5 per cent for the amount of nonylphenol produced, again based on the amount of ethoxylate released. Applying the same adjustment, a value of 1.56 per cent is used here for styrenated phenol.

To obtain values for the individual components, it is assumed that styrenated phenol produced by the degradation of ethoxylates has the same composition as was used to make the ethoxylate, product B.

The values above were applied to regional and continental emissions of ethoxylates, and also to local emissions from wool treatment. For the use in agrochemicals, a worst case assumption of complete degradation to styrenated phenol was applied. The resulting estimates of emissions are shown in Table 3.3 and Table 3.4.

Table 3.3 Regional emissions of styrenated phenol from ethoxylate (t/year).

	Wastewater	Surface water	Agricultural soil
Total emissions of ethoxylates	73	28	677
Converted to styrenated phenol	1.13 – to surface water 9.2 – to soil	0.44	11
Total as styrenated phenol		1.57	20

Table 3.4 Continental emissions of styrenated phenol from ethoxylate (t/year).

	Wastewater	Surface water	Agricultural soil
Total emissions of ethoxylates	637	254	6,096
Converted to styrenated phenol	9.9 – to surface water 81 – to soil	4.0	95
Total as styrenated phenol		13.9	176

3.1.5 Unintentional releases

None identified to date.

3.1.6 Summary of emissions data

The majority of values estimated for individual life cycle steps are confidential, and so are only presented in the confidential annex. Combined emissions for each component are presented in Table 3.5 (regional) and Table 3.6 (continental). These were derived as described in the preceding sections. As noted, where the release was estimated as an amount of styrenated phenol, these were divided between the components according to the proportions in the commercial product as used.

Table 3.5 Regional emissions (kg/d) for styrenated phenol components.

Component	Air	Waste water	Surface water	Industrial soil	Agricultural soil
Monostyrenated phenol	0.008	0.26	1.32	1.05	1.09
Distyrenated phenol	0.002	1.35	5.29	4.09	12.5
Tristyrenated phenol	0.0003	4.05	6.77	4.09	38.1

Table 3.6 Continental emissions (kg/d) for styrenated phenol components.

Component	Air	Waste water	Surface water	Industrial soil	Agricultural soil
Monostyrenated phenol	0.075	0.52	11.7	9.3	9.7
Distyrenated phenol	0.014	1.81	47.2	36.5	112
Tristyrenated phenol	0.003	4.88	60.2	36.5	340

These values were used in EUSES (European Union System for the Evaluation of Substances – software tool in support of the TGD on risk assessment) to calculate the regional and continental concentrations. The TGD and EUSES assume as a default that 80 per cent of releases to wastewater on these scales go to a wastewater treatment plant, and the other 20 per cent go direct to surface water. For this assessment, releases from the production of rubber and surfactants are assumed to go entirely to wastewater. For the other life-cycle steps, the default is applied to the wastewater releases. This is taken into account in the tables above.

3.2 Environmental fate and distribution

This section of the report reviews the fate and distribution of styrenated phenol in the environment. The information presented was derived from both predicted/calculated and measured values.

Environmental fate and distribution data were determined for each of the three components of the commercial product. Values for the physicochemical characteristics of the three components are taken from Table 1.2. Where measured values exist, these were used in preference to the predicted data.

3.2.1 Atmospheric degradation

No experimental data were available on the reaction of styrenated phenol with atmospheric photo-oxidants.

The rate constants for the reaction for each of the three components of styrenated phenol with atmospheric hydroxyl radicals were estimated using EPIWIN (v3.12) (USEPA, 2004). The overall OH rate constants are given in

Table 3.7. Half-lives are also included in the table. These values were calculated using a daily average OH radical concentration of 5×10^5 molecule cm^{-1} as in the TGD (EC, 2003).

Table 3.7 Estimated values for atmospheric oxidation of styrenated phenol.

Component	Overall oxidation rate constant (cm^3/molecule-second)	Atmospheric oxidation half-life	
		Days	**Hours**
Monostyrenated phenol	4.7×10^{-11}	0.34	8.2
2,4-Distyrenated phenol	6.2×10^{-12}	0.26	6.2
2,6-Distyrenated phenol	6.2×10^{-11}	0.26	6.2
Tristyrenated phenol	3.8×10^{-11}	0.42	10.1

All three components have short half-lives and degradation in air is expected to be rapid. However, as described in Section 3.2.7, for the two main components (di- and tristyrenated phenol) the amount in air is estimated to be low, so degradation in air will not be important overall. It may be more significant for the monostyrenated comment.

3.2.2 Aquatic degradation

Abiotic degradation

As styrenated phenol is an antioxidant it is susceptible to abiotic degradation through oxidative processes. Information from studies with other antioxidants indicates that such compounds undergo some (but not extensive) degradation in the environment (see for example Environment Agency, 2008).

Lange (2006) carried out a hydrolysis-oxidation test on distyrenated phenol over a period of 28 days according to OECD Test Guideline No. 111, 2004. The test was conducted in the dark. The purity of the test substance was 97.21 per cent. The study was conducted under four different test conditions: buffer solution at pH 7 saturated with nitrogen; algal test medium saturated with nitrogen; buffer solution at pH 7 saturated with oxygen; and algal test medium saturated with oxygen. The ratio of 2,4- and 2,6-distyrenated phenol is not given in the test report. However, analyses of both isomers were performed via high performance liquid chromatography (HPLC). The test item was found to be minimal-to-slightly eliminated over the study duration and half-lives of 95 days (pH 7/N_2) and 315 days (pH 7/O_2) were estimated. The presence of oxygen was found to have no influence on the degradation behaviour of the test item. No additional peaks were found over the study duration which indicated that no detectable degradation products were formed. Absorption to the vessel surface is not considered likely to contribute significantly to the removal seen, as differing degrees of removal were observed under differing exposure conditions.

Reaction rate constants and half-lives for distyrenated phenol were calculated despite minimal elimination of the test substance over the duration of the study. These values are highly estimated and should be treated as such. Rate constants and half-lives are summarised in Table 3.8.

Table 3.8 Estimated reaction rate constants and half-lives for distyrenated phenol (Lange, 2006).

	Buffer solution pH 7/N_2	Buffer solution pH 7/O_2	Algal medium/N_2	Algal medium/O_2
Reaction rate constant (s^{-1})	8.44×10^{-8}	2.55×10^{-8}	2.56×10^{-8}	3.86×10^{-8}
Half-life (hours)	2281	7549	7520	4987
Half-life (days)	95	315	313	208

Styrenated phenol is an antioxidant which means by definition it will react with oxidants in the environment. A number of such oxidants are known to occur in surface waters - the two most relevant being hydroxyl radicals and peroxy radicals. The rate constants for the reactions of styrenated phenol with these oxidant species are not known.

An estimate of the significance of some of the processes can be considered using generic information. Mill (1999) reported that phenols may undergo oxidation reactions with peroxy radicals ($RO_2^{\cdot}$) and hydroxyl radicals ($HO^{\cdot}$) at rates constants of 1×10^3-1×10^5 and 1-2×10^{10} respectively. The work estimated a generic half-life for phenols of 13 days via reaction with these species. This estimate was based on daily average concentrations of the reactive species under clear skies at latitudes between 40° and 50° north in the US.

Although these cannot be considered as representative of the UK or EU environment, they do suggest that oxidation may represent a notable removal process for styrenated phenol in the aquatic environment. The estimated half-life is shorter than the experimental results, but the experiments were carried out in the dark. Radical species form in natural waters as a result of the action of light; hence the experiments did not include the reactions discussed above on which the half-life of 13 days is based.

At present, given there are no experimental data to consider photo-iniated oxidiation of styrenated phenol, this approach is not considered sufficiently specific to the substance, or to the UK/EU, to be used in the calculation of environmental concentrations. Therefore no degradation by this route is included in PEC calculations. The possible significance of such degradation is considered in the risk characterisation.

Photolysis

No information was identified on the photolysis of styrenated phenols in water.

Biodegradation

Information on the biodegradation of styrenated phenol in the environment is limited. Aerobic biodegradation in activated sludge is reported to result in just seven per cent biodegradation after 28 days (Bayer, 1990a, IUCLID, 2000). The test was carried out in compliance with OECD Test Guideline 301C modified according to the EU test "Assessment of Biodegradability of Chemicals in Water by Manometric Respirometry" according to good laboratory practice (GLP). The purity and composition of the test substance was not reported and nominal concentrations were used for the tests. It was concluded that styrenated phenol (Vulkanox SP) is not readily biodegradable.

Sorption of the styrenated phenol to organic matter in the activated sludge may mean that the limited biodegradation observed is a consequence of the limited bioavailability of the compound to the microorganisms present, and not a result of any inherent resistance of the chemical itself to biological processes.

It is likely that any biodegradation that does occur will be associated with the monostyrenated component. The lower molecular weight and K_{ow} of this component compared to the di- and tristyrenated phenols mean that the monostyrenated form is likely to be relatively more bioavailable.

The BIOWIN program (USEPA, 2004) provides predictions of biodegradability for the three components (Appendix 2). All three are predicted to be not readily biodegradable.

The guidance document for PBT assessment (ECHA, 2008a) includes screening criteria for persistence based on the results of BIOWIN calculations. The criteria are:

if BIOWIN 2 <0.5 and BIOWIN 3 <2.2

or BIOWIN 6 <0.5 and BIOWIN 3 <2.2,

then the substance is considered to be persistent. The values calculated for the components of styrenated phenol are given in Table 3.9 as follows.

Table 3.9 Summary of BIOWIN predictions for styrenated phenol.

Component	BIOWIN 2	BIOWIN 3	BIOWIN 6
Monostyrenated phenol	0.97	2.76	0.21
Distyrenated phenol	0.99	2.48	0.03
Tristyrenated phenol	0.99	2.20	0.003

None of the values for BIOWIN 2 are below 0.5, so the first part of the criteria does not apply. For monostyrenated phenol, the value for BIOWIN 6 is below 0.5 but the BIOWIN 3 result is above 2.2, so this component is not considered persistent. For distyrenated phenol, the BIOWIN 6 result is below 0.5; the BIOWIN 3 value is above 2.2 but in the range 2.2 to 2.7, where the guidance recommends that cases be carefully examined. The value of BIOWIN 3 for tristyrenated phenol is just below 2.2 (the value rounds up to 2.20) and the value for BIOWIN 6 is below 0.5, indicating that this component should be considered persistent.

No information is available on the degradation of styrenated phenol in other media, nor on levels in the environment.

3.2.3 Degradation in soil

No information is available on the degradation of styrenated phenol in soil. For the reasons discussed above, any biodegradation that does occur is likely to be associated with the monostyrenated component. Photodegradation is not likely to be an important process in soil, and only the surface layer will be exposed.

3.2.4 Evaluation of environmental degradation data

Abiotic degradation of the components is concluded to occur in air and in water through reactions with radicals and oxidising species. The half-lives for these processes are set out in the preceding sections.

The compound is considered not readily biodegradable in activated sludge (wastewater treatment plants), but is likely to undergo some degradation in surface waters. On the basis of the information available, and the approaches taken in studies of other antioxidants where slightly more information was available (Environment Agency, 2005b and 2008), styrenated phenols are considered 'non-readily biodegradable' in wastewater treatment systems, and 'inherently biodegradable' in surface water, soil and sediment. The resulting biodegradation rate constants are presented in Table 3.10.

Table 3.10 Biodegradation rate constants and half lives.

Component	Water		Sediment		Soil	
	Rate (d^{-1})	Half-life (days)	Rate (d^{-1})	Half-life (days)	Rate (d^{-1})	Half-life (days)
Monostyrenated phenol	4.7×10^{-3}	150	2.3×10^{-4}	3,000	2.3×10^{-3}	300
Distyrenated phenol	4.7×10^{-3}	150	2.3×10^{-6}	3×10^{5}	2.3×10^{-5}	3×10^{4}
Tristyrenated phenol	4.7×10^{-3}	150	2.3×10^{-7}	3×10^{6}	2.3×10^{-6}	3×10^{5}

3.2.5 Adsorption

No measured values for the adsorption of styrenated phenol are available.

Values for K_{oc} can be estimated from log K_{ow} using the QSAR for soil and sediment sorption for phenols, anilines, benzo-nitriles and nitrobenzenes given in the TGD (2003) (log $K_{oc} = 0.63 \times \log K_{ow} + 0.90$). The measured log K_{ow} values were used for di- and tristyrenated phenol, the calculated value for monostyrenated phenol.

The organic carbon-water partition coefficient (K_{oc}) can also be estimated from the chemical structure of each of the components of styrenated phenol using EPIWIN.

The values predicted by these methods are presented in Table 3.11.

Table 3.11 Estimated log K_{oc} for individual components of styrenated phenol.

Component	Log K_{ow}	Log K_{oc}	
		TGD predictions	EPIWIN predictions
Monostyrenated phenol	3.67	3.20	4.50
Distyrenated phenol	**6.24**	4.83	6.56
Tristyrenated phenol	**7.8**	5.81	8.63

Measured values in bold.

The predicted values from the TGD method are used in the assessment. Solid-water partition coefficients for sediments and soils calculated from these according to the TGD are in Table 3.12.

Table 3.12 Partition coefficients for sediments and soils.

Component	Solid-water partition (l/kg)[1]					
	Soil (Kp_{soil})	Sediment ($Kp_{sediment}$)	Suspended sediment (Kp_{susp})	Soil-water partition ($K_{soil\text{-}water}$) (m^3/m^3)	Sediment-water ($K_{sed\text{-}water}$) (m^3/m^3)	Suspended matter-water ($K_{susp\text{-}water}$) (m^3/m^3)
Monostyrenated phenol	33	81	163	49	42	42
Distyrenated phenol	1.4×10^3	3.4×10^3	6.8×10^3	2.0×10^3	1.7×10^3	1.7×10^3
Tristyrenated phenol	1.3×10^4	3.3×10^4	6.5×10^4	2.0×10^4	1.6×10^4	1.6×10^4

[1] Values calculated using the default organic carbon contents for soil-water, sediment-water and suspended matter-water as specified in the TGD, 2003.

The values indicate high sorption for di- and tristyrenated components and moderate sorption for the monostyrenated component. The latter may be underestimated, as the log K_{ow} is calculated and may underestimate the actual value (Section 1.3.7).

3.2.6 Precipitation

Styrenated phenol is likely to be susceptible to deposition from the atmosphere, through wet and dry deposition and by dissolution in the rain water. The relatively high log K_{ow} values of all three components indicated that sorption to particulate matter in the atmosphere and subsequent wet or dry deposition will be an important transport process. However, the relatively low vapour pressure of all three components means that emissions to air and concentrations in air are likely to be low. This will limit the quantity of styrenated phenol available for precipitation from the atmosphere.

3.2.7 Environmental distribution modelling

The potential environmental distribution of the components of styrenated phenol has been studied using a generic level III fugacity model. The physico-chemical properties used and the results of the modelling exercise are shown in Table 3.13, Table 3.14 and Table 3.15. The model used was a four-compartment model (EQC version 1.01[13], May 1997) that has been circulated for use within the OECD HPV programme. The model was run four times with a nominal release rate of 1,000 kg/hour initially entering the air, soil or water compartments and the same release to all three.

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[13] Available from http://www.trentu.ca/academic/aminss/envmodel/welcome.html.

Table 3.13 Results of generic level III fugacity model for monostyrenated phenol.

Input data	Value				
Vapour pressure	6.5×10^{-3} Pa at 25°C				
Water solubility	231 mg/l				
Log K_{ow}	3.67				
Atmospheric half-life	8.2 hours				
Half-life in water	12 days				
Half life in sediment	3,000 days				
Half-life in soil	300 days				
Emission rate	**Model results at steady state**				
	Amount in air (%)	**Amount in water (%)**	**Amount in soil (%)**	**Amount in sediment (%)**	**Overall residence time/persistence**
Release to air	0.24	0.51	99.2	0.10	122 days
Release to water	<0.01	84	0.14	15.9	14.5 days
Release to soil	<0.01	0.16	99.8	0.03	408 days
Release to all three	0.05	2.47	97.0	0.47	181 days

Table 3.14 Results of generic level III fugacity model for distyrenated phenol.

Input data	Value				
Vapour pressure	2.57×10^{-6} Pa at 25°C				
Water solubility	0.665 mg/l				
Log K_{ow}	6.24				
Atmospheric half-life	6.2 hours				
Half-life in water	12 days				
Half life in sediment	3×10^5 days				
Half-life in soil	3×10^4 days				
Emission rate	**Model results at steady state**				
	Amount in air (%)	**Amount in water (%)**	**Amount in soil (%)**	**Amount in sediment (%)**	**Overall residence time/persistence**
Release to air	<0.01	<0.01	99.7	0.3	7,583 days
Release to water	<0.01	1.6	0.02	98.4	560 days
Release to soil	<0.01	<0.01	99.8	0.2	3.9×10^4 days
Release to all three	<0.01	0.02	98.6	1.36	1.6×10^4 days

Table 3.15 Results of generic level III fugacity model for tristyrenated phenol.

Input data	Value				
Vapour pressure	8.7×10^{-10} Pa at 25°C				
Water solubility	0.0086 mg/l				
Log K_{ow}	7.8				
Atmospheric half-life	10.1 hours				
Half-life in water	12 days				
Half life in sediment	3×10^{5} days				
Half-life in soil	3×10^{6} days				
Emission rate	**Model results at steady state**				
	Amount in air (%)	**Amount in water (%)**	**Amount in soil (%)**	**Amount in sediment (%)**	**Overall residence time/persistence**
Release to air	<0.01	<0.01	99.8	0.2	5.3×10^{4} days
Release to water	<0.01	0.88	<0.01	99.1	835 days
Release to soil	<0.01	<0.01	99.8	0.2	2.1×10^{5} days
Release to all three	<0.01	<0.01	99.5	0.5	8.8×10^{4} days

The results for monostyrenated phenol show that releases to air or to soil tend to accumulate mainly in the soil, while releases to water are found in the water and sediment. For both di-and tristyrenated phenol, releases to air and soil go to soil, while releases to water move to the sediment. This pattern largely reflects the high sorption calculated on the basis of the high log K_{ow} values for the higher styrenated components, combined with their lower solubilities, and the low vapour pressures for all components. The overall residence time increases with the degree of styrenation.

3.2.8 Bioaccumulation and metabolism

Measured data

A dietary bioaccumulation study with rainbow trout (*Oncorhynchus mykiss*) was carried out with styrenated phenol (Scheerbaum 2008). The substance tested was a mixture of distyrenated phenol (40 per cent by weight) and tristyrenated phenol (60 per cent by weight) chosen to be comparable to the commercial products. The distyrenated phenol had a purity of 99.02 per cent and the tristyrenated phenol had a purity of 96 per cent.

The study consisted of a 10-day uptake period, during which the fish were fed a diet spiked with the test substance, followed by a 42-day depuration period where the fish were fed uncontaminated diet. A control group of fish were fed uncontaminated diet over the entire test period. A positive control group was also included. This group was fed a diet spiked with a known bioaccumulative substance (hexachlorobenzene) during the uptake phase followed by uncontaminated diet during the depuration phase.

The spiked food was prepared as follows. Distyrenated phenol (57.6 mg) and tristyrenated phenol (86.4 mg) were added to 10 ml of solvent (methyl tertiary butyl ether (MTBE)) and 7.2 ml of fish oil, shaken for 10 seconds and then added to 144 g of standard fish food (floating and/or sinking pelletised diet) in 750 µl portions. The food was mixed by hand after addition of each portion. Once all of the MTBE/fish oil solution had been added, the spiked food was mixed on a bottle roller for 10 minutes and then shaken (20 rpm) for a further hour. The MTBE was allowed to evaporate under a gentle flow of nitrogen for 24 hours and the spiked food was again shaken for a final 30 minutes. Control food and positive control food was prepared in the same way without addition of the test substance (control food) or with the addition of hexachlorobenzene in place of the test substance. The prepared food was stored under a nitrogen atmosphere at -18°C until required.

The nominal concentrations prepared were 1,000 mg/kg food for the mixture of distyrenated phenol and tristyrenated phenol and 250 mg/kg food for the hexachlorobenzene positive control. The lipid content of the food was 18.8 per cent.

The test system used was a flow-through system. One replicate was carried out per test group with each replicate consisting of 125 fish in either 140 litres of water (test substance exposure) or 110 litres of water (control and positive control group). The fish were three-months old at the start of the test and had a mean initial body weight of 1.57 g. The initial loading rates were therefore 0.57 g fish/litre/day for the group exposed to the mixture of di/tristyrenated phenol and 0.059 g fish/litre/day for the control and positive control group. A daily feeding rate of three per cent of the body weight was used during the study (the food was given at two feedings daily). The water used was maintained at a temperature of 15°C and the flow rate was such to provide three renewals per day and the dissolved oxygen concentration was maintained at not less that 60 per cent of saturation through the test. The other relevant characteristics of the water were a pH of between 7.06 and 7.70 and a hardness of 55-57 mg/l as $CaCO_3$.

The fish were observed daily for mortality, behaviour and other effects. The levels of distyrenated phenol and tristyrenated phenol in the exposed fish were determined analytically on days 0, 1, 5 and 10 of the uptake phase and days 1, 2, 4, 7, 14, 28 and 42 of the depuration phase (ten fish were analysed at each sampling point). Control fish and positive control fish were sampled using a similar regime (five fish were analysed at each time point for the control group). In addition, samples of the water phase and test and control diets were also analysed at the beginning of the test and at various times during the uptake phase. The limit of quantification of analytical methods used for fish and water was 3.96 µg distyrenated phenol/fish and 5.76 µg tristyrenated phenol/fish and 1.49 µg distyrenated phenol/l and 1.44 µg tristyrenated phenol/l respectively.

During the test the mortality in the control, positive control and test group were all below 10 per cent. No mortality was observed in the group exposed to the mixture of di/tristyrenated phenol or the control group but one fish in the positive control group (exposed to hexachlorobenzene) died on day 42 of the depuration phase. No significant non-lethal effects were evident in any of the groups.

The mean (± standard deviation) concentration of test substance measured in the diet during the uptake phase was 342 ± 50 mg/kg food for distyrenated phenol and 509 ± 110 mg/kg food for tristyrenated phenol. For the positive control, the mean concentration of hexachlorobenzene in the diet was 182 ± 25.4 mg/kg. No distyrenated phenol, tristyrenated phenol or hexachlorobenzene could be detected in the control food.

The levels of distyrenated phenol, tristyrenated phenol and hexachlorobenzene measured in the fish during the test are summarised in

Table 3.1. The gut contents of the fish sampled on day 10 of the uptake phase were analysed for the presence of distyrenated phenol and tristyrenated phenol. No test substance was detected and so no further gut analyses were carried out during the test. Similarly, no distyrenated phenol or tristyrenated phenol was detectable in the water phase on days one, five and 10 of the uptake period.

Table 3.16 Levels of distyrenated phenol and tristyrenated phenol measured in rainbow trout following exposure via the diet.

Study day	Concentration (mg/kg fish)			
	Exposed group		Control group[1]	Positive control group
	Distyrenated phenol	Tristyrenated phenol	Di- + Tri-styrenated phenol	Hexachloro benzene
Day 0	Not detected	Not detected	Not detected	Not detected
Uptake day 1	5.89	7.39	Not detected	3.4
Uptake day 5	3.95	17.4	Not detected	16.5
Uptake day 10	Not detected	21.6	Not detected	25.1
Depuration day 1	Not detected	17.1	Not detected	27.5
Depuration day 2	Not detected	14.0	Not detected	24.9
Depuration day 4	Not detected	8.04	Not detected	23.2
Depuration day 7	Not detected	13.9	Not detected	15.8
Depuration day 14	Not detected	6.71	Not detected	14.6
Depuration day 28	Not detected	3.75	Not detected	7.7
Depuration day 42	Not detected	1.61	Not detected	6.9

Not detectable – less than the limit of quantification.
[1] No hexachlorobenzene was detectable in the control group.

The results for distyrenated phenol show that the concentration in the fish reached 5.89 mg/kg fish after one day of exposure but then there was a rapid decrease in the concentration in fish leading to undetectable levels by day 10 of the uptake phase and throughout the depuration phase. This pattern of uptake is unusual as the concentration in the fish would normally be expected to increase towards a steady state value during the uptake phase. A possible explanation for the pattern seen here with distyrenated phenol is that, although the substance is taken up into the organism from food (as evidenced by the occurrence in the fish on days one and five), metabolism/clearance of the substance is also rapid after five to 10 days exposure time. Thus, by days 5-10 the rate of elimination appears to have increased from that on the first day, and becomes much higher than the rate of uptake, resulting in undetectable concentrations. Given this behaviour, it was not possible to estimate the rate of uptake or depuration of the substance. However, the data show that the biomagnification factor (BMF) for distyrenated phenol is low, probably owing to rapid metabolism. Therefore, based on these data it can be concluded that distyrenated phenol has a low potential for bioaccumulation.

The uptake and depuration pattern for tristyrenated phenol shows increasing concentrations with time over the entire exposure period followed by decreasing concentrations during the depuration period. This pattern of accumulation and depuration is in line with that normally expected in accumulation studies. Based on the data reported in

Table 3.1 Scheerbaum (2008) determined the growth corrected depuration rate constant[14,15] to be 0.038 day^{-1}. Thus, the growth-corrected depuration half-life was around 18.4 days.

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[14] The overall depuration rate constant (not growth-corrected) was 0.059 day^{-1} and the rate constant for fish growth over the depuration period was 0.021 day^{-1}.

Scheerbaum (2008) calculated the assimilation efficiency and the growth-corrected steady-state biomagnification factor (BMF) from the following equations.

$$\alpha = \frac{C_{O,depuration} \times k_{overall}}{I \times C_{food}} \times \left[\frac{1}{(1 - \exp(-k_{overall} \times t))} \right]$$

$$BMF = \frac{I \times \alpha}{k_{depuration}}$$

where α = Assimilation efficiency.

$C_{O,\ depuration}$ = The concentration in fish at time zero of the depuration phase. This was assumed to be 17.1 mg/kg fish by Scheerbaum (2008) (see discussion below).

$k_{overall}$ = Overall (not growth-corrected) depuration rate constant = 0.059 day^{-1} for tristyrenated phenol.

$k_{depuration}$ = Growth-corrected depuration rate constant = $k_{overall}$ – rate constant for growth (k_{growth}). For tristyrenated phenol $k_{depuration}$ = 0.038 day^{-1}.

I = Food ingestion rate = 0.03 g food/g fish/day (feeding rate three per cent of the body weight).

C_{food} = Concentration in food = 509 mg/kg food for tristyrenated phenol.

t = Time for the uptake phase (to start of the depuration phase). Scheerbaum (2008) appears to have used 11 days (see discussion below).

BMF = Steady-state, growth-corrected biomagnification factor.

Using these parameters Scheerbaum (2008) calculated the growth-corrected steady-state BMF for tristyrenated phenol as 0.110 and the assimilation efficiency (α) as 0.138. As the lipid content of the fish was 5.8 per cent and the lipid content of the food was 18.8 per cent, the lipid normalised BMF can be determined to be 0.355.

The above assimilation efficiency appears to have been calculated by Scheerbaum (2008) based on the measured concentration in fish of 17.1 mg/kg that was determined on day one of the depuration phase (study day 11). However, by this time one day of depuration had already occurred. It is probably more correct to estimate the assimilation efficiency based on the concentration in fish at time zero of the depuration phase. This can be estimated from the intercept of the depuration curve (plot of ln [concentration in fish] against depuration day). This concentration is given as 15.3 mg/kg fish in the test report and is slightly lower than the value assumed in the calculation of the assimilation efficiency carried out by Scheerbaum (2008) above, and is also slightly lower than the concentration measured in fish at day 10 of the uptake phase (21.6 mg/kg fish). Using the concentrations in fish of 15.3 mg/kg and 21.6 mg/kg in the above equation to represent the $C_{O,\ depuration}$ value at end of the uptake period/beginning of the depuration period, and a time period of 10 days to correspond to these values, the assimilation efficiency is estimated to be in the range 0.11 to 0.15, which is similar to the value estimated by Scheerbaum (2008). These assimilation

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[15] Scheerbaum (2008) reported an uptake rate constant of 0.1052 day^{-1}. However this may be incorrect as it appears to be taken from the slope of a plot of ln [Concentration in fish] versus time over the uptake phase (days one to ten). The slope does not equal the uptake rate constant as both uptake and depuration operate in this phase. Using an initial rate approach we estimate theuptake constant to be 0.010-0.015 day^{-1} (this method provides a crude estimate of the rate constant). Using these estimates for the update rate constant, the kinetic, growth-corrected BMF is estimated to be 0.26-0.39 (ratio of uptake rate constant and growth-corrected depuration rate constant).

efficiencies would translate to a steady-state, growth-corrected BMF of around 0.087-0.12 (or 0.28-0.39 on a lipid basis).

For the hexachlorobenzene positive control, Scheerbaum (2008) determined the assimilation efficiency to be 0.507 and the steady-state, growth-corrected BMF to be 1.35. Lipid normalisation leads to a BMF of 4.42.

Overall, the study is of high quality and the results can be considered reliable. The results show that distyrenated phenol did not accumulate significantly in the study probably owing to a rapid rate of metabolism/depuration, particularly after day five of the exposure period. For tristyrenated phenol, uptake was observed but the steady-state, growth-corrected BMF was determined to be below one (BMF around 0.11 or 0.36 (lipid normalised)).

In terms of an assessment of the bioaccumulation potential of distyrenated phenol and tristyrenated phenol, the most important criterion is a bioconcentration factor (BCF) value rather than the magnitude of the BMF value. For distyrenated phenol, rapid metabolism/depuration in fish appears to be occurring. Therefore, it is concluded that the BCF for distyrenated phenol is likely to be below the threshold for a PBT-substance (well below 2,000 l/kg) and a vPvB substance (well below 5,000 l/kg).

For tristyrenated phenol, the growth-corrected depuration half-life in the fish was around 18.4 days ($k_{depuration}$ = 0.038 day^{-1}). A method for estimating BCF values from a growth-corrected depuration rate constant from a feeding study is given in the REACH Technical Guidance Document (ECHA, 2008a) as follows.

$$BCF = \frac{k_{uptake}}{k_{depuration}}$$

$$k_{uptake} = 520 \times W^{-0.32}$$

where BCF = growth corrected fish bioconcentration factor.

k_{uptake} = rate constant for uptake in fish via gills (day^{-1}).

$k_{depuration}$ = growth corrected depuration rate constant = 0.038 day^{-1} for tristyrenated phenol.

W = fish weight (g) at end of uptake/start of depuration period.

From the Scheerbaum (2008) study, the mean weight of the fish at day 10 of the uptake period was 2.36 g. Using this value in the above equation gives a value for k_{uptake} of 395 days^{-1} and an estimated growth-corrected BCF of around 10,395 l/kg. The equivalent non-growth corrected BCF would be around 6,695 l/kg. Based on these calculations it is possible that the BCF for tristyrenated phenol could be above 5,000 l/kg and so the substance should be considered as potentially vB.

While the results from the dietary study are considered valid and suitable for use in this assessment, there remains some uncertainty about the use of the REACH TGD calculation method to estimate the BCF from a BMF for a substance with log K_{ow} above six without a bioavailability correction. In Europe, Member States have agreed not to apply such a correction when considering the B/vB criteria. Further validation of this approach should be considered during the international validation of the dietary exposure method. In this case the estimated value is sufficiently above the threshold for vB that the uncertainty in the actual value does not lead to a similar level of uncertainty in the conclusion.

Calculated BCFs

The TGD (EC, 2003) provides equations for the prediction of BCF for fish, BCF for earthworms, and biomagnification factors for predators (BMF_1) and top predators (BMF_2) from log K_{ow}.

Using the TGD equations and the log K_{ow} values from Section 1.3.7, the following bioconcentration factors were calculated: for monostyrenated phenol, 263; for distyrenated phenol, 38,900; for tristyrenated phenol, 30,500.

BCF values for earthworms were calculated for di- and tristyrenated phenol. The log K_{ow} values from Section 1.3.7 were used. The results are in Table 3.27. The values calculated for the earthworm BCF are considered to have a high uncertainty, especially for log K_{ow} values above six.

Modelling of molecular dimensions suggests that none of the components trigger the exclusion criteria for bioaccumulation (ECHA, 2008b; Environment Agency, 2009).

Summary of bioaccumulation

Measured and predicted values for the bioaccumulation factors are in Table 3.27.

Table 3.27 Bioaccumulation factors for styrenated phenol (used in this assessment).

Component	Log K_{ow}	Log BCF_{fish}	BCF_{fish}	$BCF_{earthworm}$	Biomagnifcation factor	
					BMF_1	BMF_2
Monostyrenated phenol	3.67	2.42	263	57	1[a]	1[a]
Distyrenated phenol	**6.24**	nm	nm	2.09×10^4	nm	nm
Tristyrenated phenol	**7.8**	**4.02**	**10395**[b]	7.6×10^5	**0.36**	**0.36**

[a] Log K_{ow} of substance below 4.5 and BCF_{fish} below 2,000.
[b] Growth-corrected value.
Measured values in bold.
nm – no measurable uptake in feeding study.

As noted in Section 1.3.7 there is some uncertainty in the predicted log K_{ow} value for monostyrenated phenol, and this leads to uncertainty in the accumulation factors. This is considered in the assessment of exposure through the food chain (Sections 3.3.4 and 5.4.1).

The fish feeding study showed no measurable uptake of distyrenated phenol from food after five days, and it is concluded that the substance will not bioaccumulate. It is not possible to derive accumulation factors from this study, and so no calculations for exposure through aquatic food chains are made. It is also not possible to read across from fish to worms, so for distyrenated phenol the calculated BCF for earthworms is used.

The measured values for tristyrenated phenol are lower than those estimated using the TGD methods (predicted values not shown). This fits with the observation that phenolic antioxidants substances for which mammalian metabolism data are available (not included in this assessment) appear to be metabolised or excreted relatively quickly which implies that the actual potential for biomagnification for phenolic antioxidants may be lower (see for example Environment Agency, 2008). However, the measured values for fish cannot be read across to earthworms, and so the tristyrenated phenol calculated value for earthworms is used in the calculations.

3.3 Environmental concentrations

This section presents the predicted environmental concentrations (PECs) estimated to occur as a consequence of emissions from the various scenarios identified in Section 3.1 and the environmental fate and behaviour in Section 3.2.

The life-cycle steps for which local-scale emissions are relevant are listed below:

- production of styrenated phenol – negligible emissions, no PECs calculated;
- surfactant production;
- formulation of surfactants – covers formulation of products for use in agrochemicals, wool treatment and polyurethane (PU) foams;
- agrochemical use – application to soil;
- wool treatment – use of surfactants as anti-static agents;
- wool washing – removal of the anti-static treatment on subsequent washing of garments;
- PU foam stabiliser – negligible emissions, no PECs calculated;
- rubber production – use in production of E-SBR;
- tyre production – use of E-SBR containing styrenated phenol in tyres;
- article production – use of E-SBR containing styrenated phenol in rubber products other than tyres.

PECs were calculated from emission estimates for the above scenarios in accordance with the TGD, with the exception of agrochemical use, which is described later, and the following specific changes.

The production of surfactants involves the use of styrenated phenol as an intermediate, and as such a larger wastewater treatment plant (10^4 m^3/day rather than 10^3 m^3/day) and a higher dilution factor into surface water (40× rather than 10×) were used in line with the TGD. The production of rubber also involves larger amounts of water – the estimated water use for the site for which estimates are made in Section 3.1 is over 8,000 m^3/day. Accordingly, the larger treatment plant and higher dilution factor are used for this scenario as well.

For a number of life-cycle steps for tristyrenated phenol, the calculated concentration in effluent from the wastewater treatment plant is above the solubility of 7.1 µg/l as used in this assessment. In these cases, the distribution of substance in the treatment plant is adjusted to give an effluent concentration equal to the solubility, with the remainder of the substance in the sludge (no degradation and negligible volatilisation are assumed in the treatment plant).

For the marine PEC values, the default calculations assume a direct discharge to marine waters without treatment in a wastewater treatment plant. In this assessment the regeneration of styrenated phenol from ethoxylates is due to degradation of the ethoxylate in the treatment plant. Therefore, for the scenarios involving ethoxylate release (not including the agrochemical use), treatment of the effluent before discharge to marine waters is included.

All PEC values were calculated using EUSES 2.0.3[16].

3.3.1 Aquatic compartment (surface water, sediment and wastewater treatment plant)

Predicted environmental concentrations (PECs) for surface water, wastewater treatment plant effluent and freshwater sediment are shown in Table 3.38.

The only measured data relates to wastewater outputs at a styrenated phenol production site where styrenated phenol was not detected above the limit of detection (25 µg/l) (SPTF, 2007). No further comparison of measured and calculated concentrations was possible due to the lack of measured data for styrenated phenols in the environment. The calculated values were used in the risk characterisation.

The approach to estimating concentrations in water from agrochemical formulations using styrenated phenol ethoxylates was based on the calculations in the nonylphenol risk assessment, which made use of information supplied by Zeneca Agrochemicals in 1997 (ECB, 2000). This information is reproduced here, with references to nonylphenol replaced by styrenated phenol. The same assumptions apply.

As a first tier of aquatic exposure assessment, spray drift entry of pesticides, or in this case styrenated phenol ethoxylates (SPEs), into surface waters is considered. Run-off from the soil surface and leaching are not major sources of water contamination because styrenated phenol ethoxylates and styrenated phenol are strongly bound to soil (see Sections 3.1.3 and 3.2.5). When sprayed, some material may drift downwind and deposit on an adjacent surface water. The normal assumption is that application is made from a tractor-mounted boom sprayer, and the surface water onto which drift deposits is one metre downwind. The drift rate is considered to be equivalent to 2.77 per cent (PSD, 2008) of the intended application rate in the treated field. The amounts of phenol ethoxylates applied to crops are typically equivalent to 50-200 g/ha, the higher rates being used as wetters, and the lower rates as emulsifiers. In a one-metre deep water body, the resulting concentration range for the ethoxylates is given by:

C_{local} for SPEs = Applied rate × (Per cent drift/Water depth) = 0.14-0.55 µg/l

The styrenated phenol ethoxylate reaching the surface water will be readily broken down by microbial activity. Assuming instant break down to styrenated phenol (a worst-case scenario), the C_{local} range for styrenated phenol is given by the following:

C_{local} for SP = C_{local} for SPEs × (Mol weight of SP/Mol weight of SPE)

Using the information provided by industry on styrenated phenol derivatives, styrenated phenol makes up 26 per cent of the weight. Therefore:

C_{local} for SP = 0.036-0.14 µg/l

This is divided between the three components in the ratio of commercial product B and the resulting PECs are included in Table 3.18.

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[16] Available from European Chemicals Bureau, http://ecb.jrc.ec.europa.eu/

This estimate of the PEC is considered to be conservative because it assumes:

- presence of surface water one metre downwind of the treated area of the field;
- instantaneous 100 per cent conversion of ethoxylates to styrenated phenol;
- the concentration is appropriate to that at the edge of a water body (for a water body of any width the average drift entry rate will be less that the 2.77 per cent assumed here);
- no account is taken of dilution effects in flowing water bodies.

Table 3.38 PEC values for freshwater, freshwater sediment and wastewater treatment plants.

Life cycle stage	Surface water (µg/l)			Sediment (mg/kg wet weight)			Wastewater (mg/l)		
	Mono-styrenated phenol	Di-styrenated phenol	Tri-styrenated phenol	Mono-styrenated phenol	Di-styrenated phenol	Tri-styrenated phenol	Mono-styrenated phenol	Di-styrenated phenol	Tri-styrenated phenol
Surfactant production	0.64	1.4	0.12	0.023	2.0	1.75	0.025	0.058	0.007
Surfactant formulation	0.14	1.4	0.39	0.005	2.1	5.6	0.001	0.015	0.007
Agrochemical use	0.02	0.09	0.13	8×10^{-4}	0.13	1.9	-	-	-
Wool treatment	0.14	1.3	0.39	0.005	1.96	5.6	0.001	0.01	0.009
Wool washing	0.02	0.06	0.04	7×10^{-4}	0.086	0.59	4×10^{-6}	5×10^{-5}	2×10^{-4}
Rubber production	1.43	0.06	0.03	0.05	0.091	0.48	0.057	4×10^{-4}	2×10^{-5}
Rubber tyre production	0.04	0.07	0.04	1.4×10^{-3}	0.10	0.54	2×10^{-4}	2×10^{-4}	9×10^{-5}
Rubber article production	0.06	0.09	0.04	2.2×10^{-3}	0.13	0.62	5×10^{-4}	4×10^{-4}	1.9×10^{-4}
Regional	0.018	0.05	0.03	0.001	0.16	0.96			

3.3.2 Terrestrial compartment

PECs in soil for the scenarios considered in this assessment are presented in Table 3.49. For the use of agrochemicals containing styrenated phenol ethoxylates, an application rate of 200 g/ha for the ethoxylate was assumed, as in Section 3.3.1 (no reduction for spray drift). As a worst case, complete degradation of the ethoxylate to styrenated phenol was assumed, with one application taking place per year.

Table 3.49 PEC values for soil.

Life cycle stage	Agricultural soil, 30 days (µg/kg wet weight)		
	Monostyrenated phenol	Distyrenated phenol	Tristyrenated phenol
Surfactant production	0.001	0.06	0.04
Surfactant formulation	64	4,280	14,900
Agrochemical use	0.49	34	105
Wool treatment	61	4,070	14,200
Wool washing	0.23	15	48
Rubber production	0.001	0.06	0.04
Rubber tyre production	0.26	30	33
Rubber article production	0.57	64	73
Regional	0.06	65	1,730

No measured concentrations were found, so calculated concentrations were used.

3.3.3 Atmospheric compartment

Estimated local concentrations in air during an emission episode are all below 1×10^{-5} µg/m^3; as they are so low, individual values are not included here. No reports of measured concentrations of styrenated phenol in air were identified.

3.3.4 Food chain exposure

Concentrations in freshwater fish and earthworms in agricultural soil for the assessment of secondary poisoning are presented in Table 3.. As no uptake of distyrenated phenol was seen in a feeding study with fish, no concentrations in fish were calculated for this component.

No measured data for the levels of styrenated phenol in biota were identified. Therefore, the calculated concentrations are taken forward to the risk characterisation.

Table 3.20 PEC values for food chain exposure.

Life cycle stage	Fish (mg/kg wet weight)			Earthworm (mg/kg wet weight)		
	Mono	**Di**	**Tri**	**Mono**	**Di**	**Tri**
Surfactant production	0.04	na	0.46	6×10^{-5}	0.51	51
Surfactant formulation	0.02	na	1.63	0.051	34	493
Agrochemical use	0.005	na	0.31	4×10^{-4}	0.78	54
Wool treatment	0.013	na	1.3	0.048	33	472
Wool washing	0.005	na	0.33	2×10^{-4}	0.63	53
Rubber production	0.04	na	0.31	6×10^{-5}	0.51	51
Rubber tyre production	0.007	na	0.32	2.6×10^{-4}	0.74	52
Rubber article production	0.01	na	0.31	5.1×10^{-4}	1.0	53

Mono, Di and Tri are monostyrenated, distyrenated and tristyrenated phenol respectively.
na – not applicable, no uptake seen in fish feeding study, so no concentrations calculated.

3.3.5 Marine compartment

The concentrations in marine water, marine sediment and the food chain for marine predators and marine top predators are presented in Table 3. and Table 3.22. The property values (physicochemical, degradation, accumulation) for styrenated phenol used in these calculations are the same as those used for the earlier freshwater calculations (Section 3.3.1) since there is no information to suggest any significant differences in the marine environment.

Table 3.21 PEC values for marine water and sediment.

Life cycle stage	Marine water (µg/l)			Marine sediment (mg/kg wet weight)		
	Mono	**Di**	**Tri**	**Mono**	**Di**	**Tri**
Surfactant production	0.3	3.1	5.3	0.011	4.62	75
Surfactant formulation	0.01	0.14	0.041	5×10^{-4}	0.21	0.57
Agrochemical	-	-	-	-	-	-
Wool treatment	0.01	0.13	0.041	5×10^{-4}	0.20	0.57
Wool washing	0.002	0.006	0.005	6×10^{-5}	0.009	0.076
Rubber production	0.68	0.024	0.006	0.025	0.036	0.083
Rubber tyre production	0.004	0.014	0.01	1.5×10^{-4}	0.021	0.14
Rubber article production	0.007	0.025	0.015	2.6×10^{-4}	0.037	0.22
Regional	1.7×10^{-3}	0.005	0.005	7.5×10^{-5}	0.015	0.13

Mono, Di and Tri are monostyrenated, distyrenated and tristyrenated phenol respectively.

Table 3.22 PEC values for marine food chain exposure.

Life cycle stage	Marine fish (mg/kg wet weight)			Marine predator (mg/kg wet weight)		
	Mono	Di	Tri	Mono	Di	Tri
Surfactant production	0.016	na	9.2	0.003	na	2.5
Surfactant formulation	0.002	na	0.17	7×10^{-4}	na	0.09
Agrochemical	-	-	-	-	-	-
Wool treatment	0.001	na	0.14	6×10^{-4}	na	0.08
Wool washing	5×10^{-4}	na	0.04	5×10^{-4}	na	0.06
Rubber production	0.017	na	0.04	0.004	na	0.06
Rubber tyre production	7.3×10^{-4}	na	0.06	5.1×10^{-4}	na	0.06
Rubber article production	0.001	na	0.05	5.8×10^{-4}	na	0.06

Mono, Di and Tri are monostyrenated, distyrenated and tristyrenated phenol respectively.

na – not applicable, no uptake seen in fish feeding study, so no concentrations calculated.

These calculations assume there is no treatment of effluent in a wastewater treatment plant before discharge to the marine environment. This may not be the case for actual sites. For example, the major surfactant producer in the EU does not discharge directly or indirectly to the marine environment; all the wastewater from rubber production in Germany is reported to be treated before discharge (Wirtschaftsverband der Deutschen Kautschukindustrie E. V. (WDK), 2004). The majority of tyre production sites in the EU do not have marine discharges (ETRMA, 2009). Hence actual concentrations are expected to be lower in most cases. The calculations are used to indicate possible levels if such discharges do occur without a wastewater treatment plant (WWTP).

No measured levels relevant to the assessment of the marine compartment were found. Therefore, calculated levels were taken forward to the risk characterisation.

4 Effects assessment

4.1 Aquatic compartment (including sediment)

The following sections review the available toxicity data with aquatic organisms. Where possible, a validity marking is given for each study (this appears in the summary tables within each section). The following validity markings were used:

1. **Valid without restriction**. The test is carried out to internationally recognised protocols (or equivalent protocols) and all or most of the important experimental details are available.
2. **Use with care**. The test is carried out to internationally recognised protocols (or equivalent protocols) but some important experimental details are missing, or the method used, or endpoint studied, in the test means that interpretation of the results is not straightforward.
3. **Not valid**. There is a clear deficiency in the test that means that the results cannot be considered valid.
4. **Not assignable**. Insufficient detail is available on the method used to allow a decision to be made on the validity of the study.

Information on the toxicity of styrenated phenols to the aquatic compartment is limited. The only data sources identified were IUCLID (2000) and unpublished studies by industry and organisations. No information was found in the wider scientific literature.

4.1.1 Toxicity to fish

The short-term toxicity of styrenated phenol to the zebra fish *Brachydanio rerio* (now *Danio rerio*) was investigated in a 96-hour static test. LC_0 and LC_{100} (lethal concentration) values of 1 mg/l and 10 mg/l, respectively, and an LC_{50} of 3.2 mg/l (geometric mean value), have been reported (IUCLID, 2000). These results are the same as those reported in a study carried out by Bayer (1990b) using the commercial product Vulkanox SP. It is thought they are from the same study. The test was conducted in compliance with test guideline UBA-Verfahrensvorschlag “Letale Wirkung beim Zebrabaerbling Brachydanio rerio” (LC_0, LC_{50} and LC_{100}: 48-96 Studen, May 1984) according to good laboratory practice (GLP). Concentrations of styrenated phenol in the test were above the level of solubility. To achieve target concentrations, the required amount of material was weighed into water and homogenized in an Ultra-Turrax unit for 60 seconds at 8,000 revolutions per minute. At all concentrations, undissolved chemical (in the form of oily droplets) was observed on the surface of the test medium. LC_0 and LC_{100} values were determined directly from the test and the LC_{50} was calculated. Analytically determined concentrations were found to be lower than nominal values (under 80 per cent). Consequently, only the soluble fraction was taken into account. There was some deviation from the temperature range recommended by the test guideline, and the composition and purity of the test substance was not given. The study is assigned a validity score of 2/3. The presence of undissolved material makes the result difficult to interpret and not suitable for use in the assessment.

Fish were exposed to a saturated solution of di- and tristyrenated phenol (made by adding 100 mg of substance, composition 80 per cent tri- and 20 per cent distyrenated phenol to a litre of water) in a static system (Institut National de L’Environnement

Industriel et des Risques (INERIS), 1997a). No mortality was seen over 96 hours, indicating that the substance is not toxic up to its solubility. A summary of this test was seen; as the result was not suitable for use in deriving a PNEC, the full test report was not requested and no validity mark was assigned.

The Japanese Chemical Risk Information Platform (CHRIP, 2009) contains results of test on medaka (*Oryzias latipes*) for distyrenated phenol (as CAS number 2769-94-0, the 2,4- isomer) and tristyrenated phenol. The same values are given for both substances: 96-hour LC_{50} 5.6 mg/l; 14-day LC_{50} 3.8 mg/l; 14-day NOEC (no observed effect concentration) 1.9 mg/l. No details of the methods used are available. The tests were conducted in 1997. All values are above the solubilities of the substances based on the discussion in Section 1.3.5. In view of this, the lack of information on the studies and the uncertainty over the substance tested, a validity mark of four is assigned, and the results are not used in the assessment.

No long-term toxicity data are available for freshwater fish.

4.1.2 Toxicity to aquatic invertebrates

Measured values of the toxicity of distyrenated phenol to aquatic invertebrates (*Daphnia magna*) have been reported (Noack, 2006a). A 21-day *Daphnia magna* reproduction test was conducted in compliance with OECD Guideline No. 211, 1998, according to GLP.

The test item was 97.21 per cent distyrenated phenol. Due to the relatively low water solubility, a direct addition water accommodated fraction (WAF) preparation technique was employed followed by low energy stirring for 48 hours. A saturated stock solution was prepared for each test substance renewal and diluted to corresponding test concentrations. Nominal test concentrations were 18.75, 37.5, 75.0, 150, 300 µg/l, based on the results of a preliminary acute immobilisation study and 16-day reproduction study. At each test concentration there were ten replicate vessels, each containing one female *Daphnia* in 50 ml test medium. Vessels were kept under conditions of 16 hours light and eight hours darkness at 18-22°C. The test solutions were renewed three times per week with feeding at least five times per week. Water quality parameters (pH, dissolved oxygen, water hardness and temperature) were determined for one control vessel and one highest test concentration vessel two to three times a week. Test concentrations were determined on days 0, 5, 12, 19 (fresh media zero hours) and days 2, 7, 14, 21 (old media 24 hours) by high performance liquid chromatography (HPLC) using replicates prepared without test organisms (one vessel per test concentration) and stored under test conditions.

Recovery rates (RR) of measured to nominal test concentrations ranged from 49 to 119 per cent. Mean recovery rates for each test concentration ranged between 76 (nominal 37.5 and 75 µg/l) and 107 per cent (nominal 300 µg/l). NOEC, LOEC (lowest observed effect concentration) and EC_{50} values were based on measured concentrations (20.1, 35.7, 56.9, 115, 249 µg/l).

No statistically significant effects were observed in the lowest four test concentrations. At 249 µg/l, a 73 per cent reduction in offspring production and 90 per cent effect on parent mortality was observed.

The overall conclusion from the study was a 21-day NOEC of 115 µg/l for both reproduction and parental immobilisation.

The study is considered valid and suitable for the assessment (validity marking one).

A reproduction test with *Daphnia magna* was carried out with tristyrenated phenol (Noack, 2008). The test was performed according to OECD Guideline 211 (1998), according to GLP. The test substance had a purity of 96 per cent. A saturated solution of tristyrenated phenol in water was prepared using a column elution system. The column was prepared by coating glass beads with a solution of tristyrenated phenol in dichloromethane and allowing the solvent to evaporate before adding the beads to the column. Lower homologues and impurities were removed by rinsing the column with five litres of dilution water. The test water was prepared by circulating two litres of dilution water in the column for 96 hours in a closed circuit.

The beakers used for the exposures were coated for 24 hours before the test using the saturated solution. Ten *Daphnia* were exposed individually to the saturated solution for 21 days, with the same number of control organisms. All were fed at least five times a week. The solutions were renewed three times each week. Water quality parameters (pH, dissolved oxygen, water hardness and temperature) were monitored regularly through the test. The concentration of tristyrenated phenol in fresh (zero hours) and old (48 hours) media was determined once a week.

Water parameters fell within the required ranges throughout the test. No statistically significant effects were observed on reproduction, adult mortality and growth. Mortality and growth in controls were within the limits of validity. Concentrations measured in the exposures ranged from 15.1 to 55 µg/l, with an arithmetic mean of 35 µg/l.

The test is considered valid (validity marking one). There is some uncertainty regarding actual exposure level, as the solubility as determined by a column elution method using double distilled water is 7.1 µg/l, and all of the measured exposure concentrations were above this value[17]. The mean measured value is also above the limit value of <25 µg/l determined by a slow stirring method at pH 6. In view of these observations the study is interpreted as showing no effects up to the solubility of the substance, which is taken as 7.1 µg/l.

Daphnia were exposed to water soluble fractions (WSF) obtained by adding 100 mg or 30 mg of a substance made up of 80 per cent tristyrenated phenol and 20 per cent distyrenated phenol to a litre of water, agitating for 48 hours, allowing to settle for two hours and filtering (INERIS, 1997b). Dilutions of these WSFs were also prepared. Exposures were conducted according to OECD test guideline 202. No significant immobilisation was seen with the WSF from the 30 mg/l preparation, or with any dilutions of this. The undiluted WSF from the 100 mg/l preparation produced 15 per cent immobilisation, but none of the dilutions showed any significant effects. The study is interpreted as demonstrating that the EC_{50} is above the water solubility. A summary of this study was reviewed; as the result was not suitable for use in deriving a PNEC, the full test report was not requested and no validity mark was assigned.

The Japanese Chemical Risk Information Platform (CHRIP, 2009) contains results of test on *Daphnia magna* for distyrenated phenol (as CAS number 2769-94-0, the 2,4-isomer) and tristyrenated phenol. The same values are given for both substances: 48-hour EC_{50} 4.6 mg/l; 21-day reproduction EC_{50} 1.5 mg/l; 21-day reproduction NOEC 0.2 mg/l. No details of the methods used are available. The tests were conducted in 1997. All values are above the solubilities of the substances based on the discussion in Section 1.3.5, with the exception of the NOEC (which is close to the value obtained for distyrenated phenol above). In view of this, the lack of information on the studies and the uncertainty over the substance tested, a validity mark of four is assigned, and the results are not used in the assessment.

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[17] The nature of the Elendt M4 medium used in the *Daphnia* test (including pH of 7.4 to 8, and total hardness above 150 mg/l) may have contributed to this difference.

4.1.3 Toxicity to aquatic algae

The Japanese Chemical Risk Information Platform (CHRIP, 2009) contains results of test on *Selenastrum capricornutum* (now *Pseudokirchneriella subcapitata*) for distyrenated phenol (as CAS number 2769-94-0, the 2,4- isomer) and tristyrenated phenol. The same values are given for both substances: 72-hour growth rate EC_{50} above 10 mg/l; 72-hour growth rate NOEC 3.2 mg/l. No details of the methods used are available. The tests were conducted in 1997. Both values are above the solubilities of the substances based on the discussion in Section 1.3.5. In view of this, the lack of information on the studies and the uncertainty over the substance tested, a validity mark of four is assigned, and the results are not used in the assessment.

The Rubber and Plastics Additives Panel submission to the USEPA HPV Challenge programme (RAPA, 2001) proposed no testing for this endpoint on the grounds that it was appropriately covered by QSAR prediction.

4.1.4 Quantitative structure–activity relationships (QSARs)

The toxicity of styrenated phenol to aquatic organisms was predicted using ECOSAR v0.99h estimation software. Full details of the calculations, including validity ranges for these QSARs, are given in Appendix 2. The key results are summarised in Table 4.1. The predictions use equations for phenols, which are assumed to act by a polar narcosis mechanism.

QSAR estimates were determined for each of the three components of the commercial product. Calculated log K_{ow} values were used in the estimates, as the equations were developed using predicted rather than measured log K_{ow} values (Section 1.1).

Table 4.1 Summary of ECOSAR predictions for the toxicity of styrenated phenol to aquatic organisms (mg/l).

Component	96h-LC_{50} for fish	48h-LC_{50} for *Daphnia*	96h-EC_{50} for green algae	30d-NOEC[1] for fish	21d-NOEC for *Daphnia*	96h-NOEC for green algae
Mono-styrenated phenol	2.726	2.214	3.276	0.28	0.21	0.61
Distyrenated phenol (2.4-isomer)	0.194	0.442	0.061	0.019	0.015	0.04
Distyrenated phenol (2,6-isomer)	0.649	0.984*	0.346	0.066	0.05	0.14
Tristyrenated phenol	0.041*	0.175*	0.006	0.004	0.004	0.008*

[1] NOEC values derived from predicted ChV values by dividing by √2. ChV (Chronic value) taken as the geometric mean of the NOEC and LOEC.

*Chemical may not be soluble enough to measure this predicted effect.

The TGD also provides equations to calculate toxicity values from the log K_{ow} value, and the results are in Table 4.2.

Table 4.2 Predicted toxicity values using TGD equations (mg/l).

Component	96h-LC_{50} for fish	48h-LC_{50} for *Daphnia*	96h-EC_{50} for green algae	Fish 28-32d NOEC	*Daphnia* 16d NOEC (growth)
Mono-styrenated phenol	6.13 (2.87)	3.1 (2.83)	2.5	0.50	0.39
Distyrenated phenol	0.061 (0.058)	0.017 (0.160)	0.010	0.004	0.001
Tristyrenated phenol	0.004 (0.006)	8.1×10^{-4} (0.028*)	4.1×10^{-4}	2.1×10^{-4}	4×10^{-5}

* Chemical may not be soluble enough to measure this predicted effect.
Values in ( ) calculated using polar narcosis equations; other values calculated using non-polar equations.

For these TGD calculations, the measured log K_{ow} value was used where possible as the equations were derived using measured values. In the absence of measured data, a calculated log K_{ow} was used for monostyrenated phenol. The equations used were those for non-polar narcosis. As phenols, the components of styrenated phenol could be considered to act by a polar narcosis mechanism. Calculations for this mechanism were only possible for acute toxicity to fish and *Daphnia*; these values are also included in Table 4.2. It is possible that at the high log K_{ow} values of the two higher styrenated components, the additional toxicity for this mechanism is not expressed[18].

Both methods have limited reliability at higher log K_{ow} values, especially for values as high as that for tristyrenated phenol.

4.1.5 Endocrine disruption

Styrenated phenol is not listed on the EU candidate list of endocrine disruptors[19].

Ogawa *et al*. (2006) presented the results of screening tests for estrogenic activity using a yeast two-hybrid assay. Styrenated phenol with three different compositions was among the antioxidants tested.

A mixture of mono- (74 per cent) and distyrenated phenol (26 per cent) showed the strongest activity of the three. The authors considered this activity comparable o activity observed for nonylphenol and bisphenol A.

A mix of mono-, di- and tristyrenated phenol of unknown composition showed a lower activity, and a mixture of 93 per cent di- and seven per cent tristyrenated phenol showed no activity unless treated with rat liver S-9 to generate metabolites. The authors presumed that monostyrenated phenol played the predominant role in the activity seen.

The OECD (Q)SAR toolbox (OECD, 2008) includes an estrogen receptor binding profiler tool. The method employs a 'four phase' assessment that includes Comparative Molecular Field Analysis (CoMFA) and the Common Reactivity Pattern Approach (COREPA). This gives the following results for the components of styrenated phenol. The monostyrenated phenol isomers are indicated to be moderate binders. The 2,4-distyrenated phenol isomer is indicated to be a strong binder. The 2,6-distyrenated

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[18] In fact,predictions using polar narcosis equations give a lower toxicity to *Daphnia* than those using non-polar equations for di- and tristyrenated phenol; in these circumstances lower values would be used.

[19] http://europa.eu.int/comm/environment/docum/pdf/bkh_annex_01.pdf.

phenol isomer and tristyrenated phenol are identified as having hindered phenol groups, suggesting a lower binding activity.

These effects are not considered further at this time but in view of the effects shown by some other substituted phenols, further investigation may be required in future work.

4.1.6 Wastewater treatment plant microorganisms

A three-hour EC_{50} value of 362 mg/l was reported for the toxicity of styrenated phenol to microorganisms in activated sludge, based on the inhibition of oxygen consumption (IUCLID, 2000). The same result was reported in a test carried out by Bayer (1990c) and it is thought to be the same study. The test was conducted to GLP using method ISO 8192 ‘Test for inhibition of oxygen consumption by activated sludge’ using the commercial product Vulkanox SP. The composition and purity of the test substance was not given and analytical monitoring was not carried out. The study is assigned a validity rating of two; although few details are available, these are considered sufficient to use the result in the assessment.

4.1.7 Toxicity to sediment organisms

No data was identified on the toxicity of styrenated phenols to sediment organisms.

4.1.8 Predicted no-effect concentrations for the aquatic compartment

Calculation of a PNEC for surface water

The PNEC for surface water is the concentration at which, or below which, exposure is considered not to present a significant risk to the aquatic environment. It is calculated by dividing the lowest short-term median lethal (effect) concentration, $L(E)C_{50,}$ or long-term NOEC value by an appropriate assessment factor. The assessment factor applied depends on the size and suitability of the toxicity dataset available.

A measured NOEC of 115 µg/l was determined for the distyrenated component for *Daphnia* (Noack, 2006a) and no effects were seen at solubility in a long-term *Daphnia* test with the tristyrenated component (Noack, 2006b). These are the only measured values considered to be reliable. Acute $L(E)C_{50}$ and long-term toxicity ChV (chronic) values were estimated using ECOSAR (v3.12). NOEC values were derived from the predicted chronic (ChV) values by dividing by $\sqrt{2}$. Acute toxicity and NOEC values were also calculated using the equations from the TGD.

Comparison between the measured and calculated values can be made only for the chronic toxicity to *Daphnia*. The relevant values for distyrenated phenol are in Table 4.3. As noted above, calculated log K_{ow} values were used with ECOSAR and measured ones (where possible) with the TGD equations. To include possible consequences from this, predictions using EPIWIN with the measured log K_{ow} values and using the TGD equations with the calculated log K_{ow} values were also made.

Table 4.3 Comparison of predicted and measured chronic toxicity values for distyrenated phenol to *Daphnia.*

Source	Log K_{ow} used	NOEC (µg/l)
Measured	-	115
EPIWIN	Calculated, 2,4-	15
	Calculated, 2,6-	50
	Calculated, composite	35
	Measured	8.5
TGD	Measured	1.2
	Calculated, 2,4-	3.2
	Calculated, 2,6-	25
	Calculated, composite	16

From this comparison, predicted values are always smaller than the measured value, in some cases by nearly two orders of magnitude. ECOSAR values are closer to the measured value than those from the TGD method, and are closer to the calculated log K_{ow} value than the measured value. In the absence of other data, predicted toxicity values using ECOSAR with calculated log K_{ow} values are used in the assessment along with the measured value. In support of this, both the di-and tristyrenated phenols fall outside of the domain of the TGD equations (as both are above six). The predicted values using ECOSAR still appear to overestimate the toxicity for invertebrates, and so may provide some degree of conservatism. There is no information to judge whether the same is true for the other taxonomic groups.

To extend the comparison, data for 4,4'-dihydroxy-2,2'-diphenyl propane were used as this has a related structure to monostyrenated phenol. The comparison uses only long-term toxicity data. Measured and predicted (ECOSAR) values are in Table 4.4. Predictions are based on the calculated log K_{ow} value, but this agreed well with the measured value.

Table 4.4 Predicted and measured chronic toxicity values for 4,4'-dihydroxy-2,2'-diphenyl propane (mg/l).

Species	Predicted	Measured
Fish	0.035	0.016 – 3.6
Daphnia	0.25	3.15
Algae	0.73	1.4

Predictions for fish and algae are in reasonable agreement with measured values. The toxicity to *Daphnia* is overestimated, as it is for distyrenated phenol. This comparison adds some support to the use of the predicted toxicity data here.

For tristyrenated phenol, the chronic test with *Daphnia* showed no effects at solubility. The NOEC value predicted by ECOSAR is around half of the solubility, which again indicates some overestimation of toxicity. The value predicted using the TGD equations is much lower.

NOEC values derived from the EPIWIN predictions are included in Table 4.5, together with measured values for di- and tristyrenated phenol[20]. In view of likely conservatism

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[20] Note that the experimental result with *Daphnia* for tristyrenated phenol has been interpreted as showing no effects at a solubility of 7.1 µg/l. As the predicted value for the algal NOEC is also above the solubility, this has also been set to a value of 7.1 µg/l for consistency.

in the predictions, they were treated as equivalent to measured values in this assessment. As there are three NOEC values for each component, an assessment factor of 10 was applied to the lowest NOEC value in each case. This is not a standard approach according to the TGD, but under REACH the use of reliable predicted values in place of measured ones is expected to become more common. The resulting PNEC values are also in the table. Water solubility values are included to show that predicted toxicity values are below the solubility.

Table 4.5 Selected long-term toxicity values and PNECs for styrenated phenol.

Component	Water solubility (mg/l)	Lowest long-term NOEC values (µg/l)[1]			PNEC (µg/l)
		Fish	Invertebrates	Algae	
Monostyrenated phenol	231	283	209	608	21
Distyrenated phenol[2]	0.665	45	**115**[3]	96	4.5
Tristyrenated phenol	0.0071	4.2	**7.1**[4]	7.1[5]	0.42

All NOEC values calculated using EPIWIN (v3.12), except for the measured values shown in bold.

[1] Derived from ChV values by dividing by √2 (except for measured value).

[2] Composite values for the mixture of the 2,4 and 2,6-distyrenated isomers.

[3] Measured value (Noack, 2006a).

[4] Based on measured data (Noack, 2006b). Interpreted as no effects at solubility (7.1 µg/l)

[5] Predicted value above water solubility, set to solubility (7.1 µg/l) for consistency.

These predictions use the calculated log K_{ow} values as described in Section 4.1.4. If the measured log K_{ow} values were used for di- and tristyrenated phenols, the resulting PNEC values would be 0.85 µg/l and 0.14 µg/l respectively.

In addition to the PNECs given here a value of 1.15 µg/l, derived from the measured value with an assessment factor of 100, is also considered for distyrenated phenol in the risk characterisation[21].

Calculation of PNEC for sediment

No information is available on the toxicity of styrenated phenol to sediment organisms. In the absence of experimental data, the PNEC for sediment was estimated using the equilibrium partitioning approach described in the TGD. The data are summarised in Table 4.6.

Table 4.6 Derived PNECs for sediment.

Component	Log K_{ow}	$K_{susp\text{-}water}$ (m^3/m^3)	PNEC for surface water (µg/l)	PNEC sediment (mg/kg wwt)
Monostyrenated phenol	3.67	41.5	20.9	0.76
Distyrenated phenol	6.24	1,700	4.5	6.6
Tristyrenated phenol	7.8	16,300	0.42	5.95

Distyrenated and tristyrenated components have a log K_{ow} above five. Therefore, as recommended in the TGD the risk characterisation ratios were increased by a factor of ten to take account of the possible ingestion of sediment-bound substance.

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[21] A factor of 10 rather than 100 could be considered if invertebrates were the most sensitive group. However, the available data do not allow a most sensitive group to be identified. Also, for phenol, nonylphenol and octylphenol the lowest NOEC value for fish is lower than the lowest for *Daphnia*. Therefore, the higher factor is used here.

Calculation of PNEC for WWTP microorganisms

The only value available for the calculation of a PNEC was the three-hour EC_{50} of 362 mg/l reported for activated sewage sludge organisms (Bayer, 1990c). Although this is in excess of the solubility of all components, exposure to mixed (dissolved and suspended) substance is considered to be relevant to this endpoint.

A PNEC of 3.62 mg/l was derived using an assessment factor of 100, in accordance with the TGD (EC, 2003). This value relates to the added commercial substance, which was of product type B. As a worst case approach, it could be assumed that the effect was due to only one component, and that this was present at the level in product type B. The resulting PNEC values are 0.40 mg/l for monostyrenated phenol, and 1.6 mg/l for di- and tristyrenated phenol. This is a worst case approach. A comparison of the overall effect level and combined concentrations of the three components was considered.

PNECs for the marine compartment

There are no data on toxicity to marine organisms for styrenated phenol or any of the components. Therefore, PNECs for marine water were derived by applying an assessment factor of 100 to the lowest NOEC from the freshwater data. The sediment PNECs were estimated by the equilibrium partition method as for freshwater. The resulting values are in Table 4.7.

Table 4.7 Marine PNEC values.

Component	PNEC for marine surface water (µg/l)	PNEC for marine sediment (mg/kg wet weight)
Monostyrenated phenol	2.1	0.076
Distyrenated phenol	0.45	0.66
Tristyrenated phenol	0.042	0.6

4.2 Terrestrial compartment

4.2.1 Terrestrial toxicity data

No relevant toxicity data for terrestrial organisms were located.

4.2.2 Calculation of PNEC for the soil compartment

In the absence of any experimental data, the PNEC for soil was calculated using the equilibrium partitioning method outlined in the TGD. Data are summarised in Table 4.8.

Because the log K_{ow} of the distyrenated and tristyrenated components is above five, the PEC/PNEC ratios were increased by a factor of ten to take into account the possible ingestion of soil-bound substances.

Table 4.8 Derived PNECs for soil.

Component	Log K_{ow}	$K_{soil\text{-}water}$ (m^3/m^3)	PNEC for surface water (µg/l)	PNEC for soil (mg/kg wet weight)
Monostyrenated phenol	3.67	49.1	20.1	0.60
Distyrenated phenol	6.24	2,030	4.5	5.38
Tristyrenated phenol	7.8	19,500	0.42	4.83

4.3 Atmospheric compartment

There are no data on the effects of styrenated phenols through aerial exposure. Direct emissions to the atmosphere are likely to be very low. The limited volatility of the individual components of the commercial product, and preferential partitioning to the solid phase means that concentrations of styrenated phenol in the atmosphere are expected to be low. Therefore, a PNEC was not derived.

4.4 Mammalian toxicity data

This section presents a review of mammalian toxicity data. The results are used in this report for the assessment of non-compartment specific effects relevant to the food chain (secondary poisoning). No human health risk assessment is included.

The toxicity of styrenated phenol has not been investigated extensively. Most studies have been conducted with poorly characterised mixtures of mono-, di-, or tristyrenated phenols. No data were identified for the toxicity of the three components individually to mammals; therefore, it was not possible to assess the toxicity of specific styrenated phenol forms.

The full study reports were assessed where available, but for the majority of studies the only information available was from IUCLID.

4.4.1 Toxicokinetics

No studies were found on the toxicokinetics of styrenated phenol. From acute and repeated dose oral studies it can be elucidated that oral absorption occurs. An absence of adverse effects following dermal administration suggests that styrenated phenol is not readily absorbed via this route. Based on their relatively high molecular weights, moderate water solubility and moderately high n-octanol-water partition coefficients, uptake by all exposure routes are predicted to be limited.

4.4.2 Acute toxicity

Only studies in experimental animals are available.

Inhalation

One acute inhalation study was described in IUCLID. Six rats were exposed to air passed through “styrenated phenol” for six hours at ambient temperature (Monsanto, 1974a). The LC_{50} was determined to be above 0.21 mg/l. No further information is available.

Oral

In a GLP-compliant OECD guideline study, female Sprague Dawley rats (five per group) were exposed via gavage at 5, 10, 20 or 40 g/kg to a mixture of tristyrenated phenol and distyrenated phenol (80/20) (Rhöne Poulenc, 1997a). Five males were also exposed to 4 g/kg. The observation period was 14 days. The top dose was administered in two treatments, three hours apart. No deaths occurred at any of the dose groups. Clinical signs included hypoactivity, piloerection, hunched posture, diarrhoea and urine stained perineum. An LD_{50} could not be determined from this study, although the findings indicate very low acute toxicity.

In an unpublished study, groups of two or three male and female Sprague Dawley rats were dosed via gavage to 2,000, 2,510, 3,160 or 3,980 mg/kg "styrenated phenol" in a 50 per cent solution in corn oil and observed for seven days (Monsanto, 1972). Deaths occurred at 2,510 mg/kg (2/5) and above (4/5 and 5/5 for 3,160 and 3,980 mg/kg, respectively). Survival time ranged from one to five days, with most deaths occurring within two days. Clinical signs included reduced appetite and activity, increased weakness and collapse. Necropsy revealed lung hyperaemia, slight liver discolouration and acute gastrointestinal inflammation. An oral LD_{50} of 2,680 mg/kg was determined.

Three further acute oral toxicity tests are briefly described in IUCLID:

"Styrenated phenol" was administered as a 50 per cent solution in corn oil to rats, which were subsequently observed for seven days (Wisconsin Alumni Research Foundation, 1956). An LD_{50} of 2,500 mg/kg body weight was determined.

"Styrenated phenol" was again administered as a 50 per cent solution in corn oil to two to three male and female rats per dose level (Monsanto, 1974b). An LD_{50} of 3,550 mg/kg body weight was determined.

No lethality occurred when 500 mg/kg "styrenated phenol" was administered to rats in a study conducted to US guidelines and to GLP (Ricerca Inc, 1993). No body weight deficits, clinical or gross anatomical changes were observed in a 14-day observation period. An LDL_0 above 500 mg/kg body weight was determined.

Dermal

Sprague Dawley rats (five per sex) were exposed to a dermal application of 5,000 mg/kg mixture of tristyrenated phenol and distyrenated phenol (80/20) in a GLP-compliant OECD guideline study (Rhöne Poulenc, 1997b). No mortality resulted and no adverse clinical signs were observed. An LD_{50} cannot be determined from this study.

One acute dermal toxicity study is reported in IUCLID (Monsanto, 1974b): One male and one female rabbit were dosed with "styrenated phenol" at each dose level. No further details are provided. A dermal LD_{50} above 7,940 mg/kg bw was determined.

Summary of acute toxicity

The acute toxicity of styrenated phenol has been investigated via the oral and inhalation routes of exposure in rats and via the dermal exposure route in rats and rabbits. Good quality studies are available for oral and dermal exposure routes, but only limited information is available for the inhalation exposure route.

No species or sex sensitivity can be determined from the information available. Styrenated phenol has been shown to be of low acute toxicity via the inhalation, oral and dermal routes of exposure.

4.4.3 Irritation

The only data available relate to experimental animals and there are no human data.

Skin

A mixture of tristyrenated phenol and distyrenated phenol (80/20) was tested for dermal irritation potential in rabbits in a study compliant with OECD guidelines and GLP (Rhöne Poulenc, 1997c). Exposure was for three minutes, one hour or four hours. Slight erythema was present in one rabbit one hour after the longest exposure period. No other signs of dermal irritation were recorded.

Two skin irritation studies in rabbits are reported in IUCLID (Bayer, 1991, Monsanto, 1974d). The first study was conducted to OECD guidelines and to GLP (no further details). In the second study 0.5 ml "styrenated phenol" was applied to intact and abraded skin for 24 hours to six albino rabbits (GLP not performed). The mean irritation score in the second study was 0.7/8.0. These findings indicate no or minimal skin irritation potential.

Eye

A mixture of tristyrenated phenol and distyrenated phenol (80/20) was tested for eye irritation potential in rabbits in a study compliant with OECD guidelines and GLP (Rhöne Poulenc, 1997d). Slight or moderate conjunctival redness (Grade 1 or 2) was present in all rabbits one hour after exposure and slight redness persisted in one animal 24 hours after exposure. No signs of irritation were observed 48 hours after exposure in any of the animals.

Two eye irritation studies in rabbits are reported in IUCLID (Bayer, 1991, Monsanto, 1974e). The first study was conducted to OECD guidelines and to GLP (no further details). In the second 0.1 ml styrenated phenol was applied for 24 hours to six albino rabbits (GLP not performed). The mean irritation score in the second study was 4/110. These findings indicate no or minimal eye irritation potential.

Respiratory Tract

No data are available on the respiratory tract irritation potential of styrenated phenol.

Summary of irritation

No evidence of skin or eye irritation was reported in acceptable studies. No data on the potential of styrenated phenol to cause respiratory irritation are available.

4.4.4 Corrosivity

No evidence of corrosivity was reported in an acceptable skin irritation study.

4.4.5 Sensitisation

Studies in animals

A Buehler skin sensitisation study in guinea pigs conducted to GLP and reportedly to OECD guidelines was completed using a mixture of tristyrenated phenol and distyrenated phenol (80/20) (Rhöne Poulenc, 1997e). Induction and challenge concentrations were both 75 per cent. No skin reactions were observed on challenge with the test substance.

A non-standard guinea pig maximisation test to determine causative agent of allergic contact dermatitis from rubber boots was performed using three groups of eight animals (3/8 were controls) (Kaniwa et al, 1992). Induction was with “rubber boot”, and two agents previously shown to be causative chemicals in rubber boot sensitisation; 2-mercaptobenzothiazole (MBT) and benzothiazyl disulfide (MBTS). Challenge was conducted with fractions of “rubber boot”. One such fraction did not cause a reaction in the MBT or MBTS groups, but did cause slight erythema in 4/5 animals after 48 hours in the “rubber boot” group. This fraction was identified to consist of di- and tristyrenated phenols.

Although a positive result on challenge with styrenated phenol in a sensitisation study was gained, a more robust study gave a clear negative result. On this basis styrenated phenol has not sufficiently been proven to be sensitising to animals.

Studies in humans

Skin

Patch testing for styrenated phenol sensitisation was performed in two patients who had rubber footwear dermatitis (Kaniwa et al, 1994). One of the subjects gave a negative result and one a positive result. No reactions were gained from thirty patients with rubber dermatitis who were patch tested for sensitisation to styrenated phenol after visiting Toho University Hospital during 1980-1982.

Although a positive result was observed in one of the patch tests, this is not sufficient to conclude that styrenated phenol is a skin sensitiser.

Respiratory tract

No data are available on the respiratory tract sensitisation potential of styrenated phenol in humans.

Summary of sensitisation

Although data indicating the sensitising potential of styrenated phenol is available, this is in the form of a non-standard maximisation test and mixed results from human patch testing. The more robust data available, a Buehler test, does not indicate that a mixture of tristyrenated phenol and distyrenated phenol (80/20) has the potential to cause skin sensitisation. No data on the potential of styrenated phenol to cause respiratory sensitisation are available.

4.4.6 Repeated dose toxicity

Only data on experimental animals are available.

Oral

Two briefly described oral repeat dose toxicity studies are reported on IUCLID.

Male and female rats were fed 5 to 500 mg/kg styrenated phenol daily for 90 days (Food and Drug Research Laboratories, 1961). No significant toxic effects were noted. Growth was retarded in both sexes in the highest dose groups and liver weights were increased (at 158 and 500 mg/kg) in the absence of any adverse histopathological or biochemical changes. The IUCLID dataset described a no observed adverse effect level (NOAEL) of 50 mg/kg and a lowest observed adverse effect level (LOAEL) of 158 mg/kg.

Male and female rats were fed 5 to 500 mg/kg styrenated phenol daily for 36 weeks (Food and Drug Research Laboratories, 1962). No significant toxic effects were noted. Growth was decreased in the highest dose groups and liver and kidney weights were increased (500 mg/kg) in the absence of any adverse histopathological or biochemical changes. The IUCLID dataset has described a NOAEL of 150 mg/kg and a LOAEL of 500 mg/kg.

No data are available on repeat dose effects through inhalation or dermal exposure.

Summary of repeated dose toxicity

The available information is limited. No significant toxicological effects were observed in two old, and briefly reported, repeat dose studies in rats. A NOAEL of 50 mg/kg and a LOAEL of 158 mg/kg are identified, based upon decreased growth and an increase in liver weight. A high level of uncertainty is associated with the NOAEL and LOAEL estimates because the studies are old and it is not possible to assess their quality given only brief descriptions.

4.4.7 Mutagenicity

In vitro studies

Bacterial studies

A mixture of tristyrenated phenol and distyrenated phenol (80/20) was tested in an OECD guideline GLP compliant Ames test using *Salmonella typhimurium* strains TA98, TA100, TA102, TA1535, and TA1537 with and without metabolic activation (Rhöne Poulenc, 1997f). Doses ranged from 50 to 5,000 µl per plate. No mutagenic activity was observed with or without the addition of metabolic activation.

Styrenated phenol was tested in an Ames test using the overlay technique (Monsanto, 1976). *Salmonella typhimurium* TA98, TA100, TA1535, TA1537, and TA1538 and *Saccharomyces cerevisiae* D4 were incubated with 0.001 to 5.0 µl per plate in DMSO in the presence and absence of metabolic activation. Only one plate per dose was used and toxicity was observed at one and five µl. Negative and positive controls were run concurrently and produced appropriate results. No increase in the number of revertants was observed for any dose or strain with or without metabolic activation. Overall, the styrenated phenol tested in this assay was non-mutagenic to bacteria.

Another Ames test and a DNA damage and repair assay are reported in IUCLID.

A negative result was gained after *Salmonella typhimurium* TA98, TA100, TA1535 and TA1537 were incubated with 0.1 to 1,000 µg/l styrenated phenol with and without metabolic activation (Goodyear Tire & Rubber Company, 1980). The study was not conducted in accordance with GLP

A positive result was gained after 10 to 100 µg/l styrenated phenol without metabolic activation was tested with E.coli Pol A+ and Pol A1 in a liquid suspension assay (Goodyear Tire & Rubber Company 1981). No further details are provided.

Mammalian cell studies

No data are available.

In vivo studies

No data are available.

Studies in humans

No data are available.

Summary of mutagenicity

Investigation of the genotoxicity of styrenated phenol is limited, having only been tested *in vitro* in three Ames tests and in *E.coli*. The genotoxicity of styrenated phenol has not been investigated further *in vitro* or *in vivo*. The limited information available does not provide any evidence to indicate genotoxic potential.

4.4.8 Carcinogenicity

A carcinogenicity study is not available. No obvious adverse effect relating to carcinogenicity was observed in studies lasting 36 weeks. Although only limited genotoxicity information is available, there is no indication that styrenated phenol is carcinogenic.

4.4.9 Toxicity for Reproduction

No studies on the reproductive toxicity potential of styrenated phenol are available. No data are available on the reproductive toxicity potential of styrenated phenol in humans.

4.4.10 Other information

A non-standard study is available which investigates the possible inhibitory activities of substances in rubber materials on intercellular gap-junction communication (Tsuchiya *et al*., 1995). Inhibition of metabolic cooperation may identify potential tumour promoters. Styrenated phenol inhibited metabolic cooperation at concentrations of 2.5 to 5 ug/ml. This is a lower inhibitory concentration than lithocholic acid (a known promoter at intestinal sites). Whilst this study demonstrates a possible tumour promoting effect, there is no direct evidence to establish it as such.

4.4.11 Summary of mammalian toxicity

No data on the toxicokinetics of styrenated phenol are available.

Acute toxicity studies demonstrated LD_{50} values for inhalation, oral and dermal routes of over 0.2 l/mg, 2,500 to 4,000 mg/kg bw and over 7,040 mg/kg bw, respectively.

Skin and eye irritation studies do not indicate that styrenated phenol has irritating properties.

The data do not indicate that a mixture of tristyrenated phenol and distyrenated phenol (80/20) has the potential to cause skin sensitisation. No data on the potential of styrenated phenol to cause respiratory sensitisation are available.

A NOAEL of 50 mg/kg and a LOAEL of 158 mg/kg are identified for repeated dose toxicity, based upon decreased growth and an increase in liver weight. A high level of uncertainty is associated with the NOAEL and LOAEL estimates because the studies are old and it is not possible to assess their quality given only brief descriptions.

Based upon negative results of the studies available, styrenated phenol is not considered to be an *in vitro* mutagen. No information on the potential of styrenated phenol to be an *in vivo* mutagen is available.

No data regarding the carcinogenic or reproductive toxicity potential of styrenated phenol are available.

Overall, for the purposes of human health risk assessment and effects of secondary poisoning, the critical health effect is repeated dose toxicity for which a NOAEL of 50 mg/kg/day has been identified in rats. A high level of uncertainty is associated with this NOAEL because of limitations in the available repeat dose toxicity studies, incomplete assessment of genotoxicity and the absence of specific reproductive toxicity data.

The uncertainties in this hazard assessment could be reduced if the scope and reliability of the repeated dose toxicity studies was assessed and genotoxicity (initially an *in vitro* chromosome aberration study and an *in vitro* mammalian cell gene mutation are required) and reproductive toxicity hazard identification testing was completed following the strategies outlined in the Technical Guidance Document on Risk Assessment (EC, 2003).

4.4.12 Derivation of $PNEC_{oral}$

The $PNEC_{oral}$ for secondary poisoning was calculated according to the methods in the TGD (EC, 2003). The lowest NOAEL was reported for a 90-day repeated dose oral feed toxicity study in rats (Food and Drug Research Laboratories, 1961). A conversion factor of 20 was applied to the NOAEL of 50 mg/kg as the trial lasted for more than six weeks. An assessment factor of 90 was also applied to give a $PNEC_{oral}$ of 11.11 mg/kg food.

This value is determined for styrenated phenol as a commercial product, as there are no toxicity data for the individual components. As such it is only comparable with concentrations of the commercial product, that is where the three components are present in the same ratios as in the product. The different transport and partitioning behaviour of the three components in the environment means they are predicted to be present in prey species in quite different ratios to the commercial products. In water, the concentrations are di > tri > monostyrenated; in soil the ratios are tri > di > monostyrenated. Therefore, a comparison of the combined concentrations with the PNEC from above does not compare like with like.

Two exploratory approaches were used to investigate the risks from secondary poisoning. In the first, the PNEC from above was compared with the combined concentrations of the components. This had the limitations described above, and is likely to underestimate the risks. For the second approach it was assumed that the toxic effect in the test was due to only one component. It is understood that the substance tested was of product type A. Hence for monostyrenated phenol, which is present at 11 per cent, the PNEC is 1.2 mg/kg food. For distyrenated phenol and tristyrenated phenol, which are present at 43 per cent, the PNEC is 4.8 mg/kg food. This is a worst case approach, and will overestimate the risks.

4.5 Mode of action

There is no information on the actual mode of action of styrenated phenols. However, it is likely that, as with other phenols, the substances act by a polar narcosis mechanism. This mode of action was assumed in the derivation of QSAR estimates for the effects data, although as noted in Section 4.1.8 the di-and tristyrenated phenols in particular may not express any excess toxicity.

4.6 Classification

4.6.1 Classification for human health

Styrenated phenol is currently not classified with respect to human health and is not listed in Annex 1 of Directive 67/548/EEC. Based on the data presented in Section 4.4, classification for health effects is not proposed.

4.6.2 Classification for the environment

Styrenated phenol is not currently classified as dangerous for the environment under the Dangerous Substances Directive (67/548/EEC).

Styrenated phenol is not readily biodegradable, and has a high potential for accumulation (log Kow values for all three components are above three). The limited data on acute aquatic toxicity indicate no acute effects up to the solubility. On this basis, the substance is not classified. However, classification as ‘Dangerous for the environment’ with the risk phrase ‘R53: may cause long term adverse effects in the aquatic environment’ could be considered on the basis of persistence and accumulation and the demonstrated chronic toxicity for the distyrenated component.

Under the new EU Classification, Packaging and Labellling Regulations[22] reliable predictions can be used in the absence of experimental data although the robustness and validity of such predictions should be assessed when applying classification.

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[22] As implemented by Regulation (EC) 1272/2008 and using the Global Harmonised System for classification (GHS).

For the mono- component, QSAR estimates indicate acute EC_{50} values within the range 1.0 to 10 mg/l, indicating this component would not have an acute category. Given the lack of ready biodegradation and that predicted chronic NOECS are below one mg/l, Chronic 2 appears applicable.

For the di- component, QSAR estimates indicate acute EC_{50} values below one mg/l and below the experimental water solubility indicating Acute 1. With the lack of ready biodegradation, Chronic 1 also appears to be applicable. Comparison of distyrenated measured chronic *Daphnia* data with predicted chronic *Daphnia* data indicates that QSAR predictions for the di- component may overestimate toxicity. On this basis, it does not seem appropriate to define an M factor.

For the tri- component, QSAR estimates indicate acute EC_{50} values for fish and algae are below the experimental water solubility and below one mg/l. There are no chronic effects on *Daphnia magna* at the limit of water solubility, however, which indicates that QSAR predictions for the tri- component may overestimate toxicity. Considering this and potential QSAR uncertainty for such low solubility, high log Kow substances, acute QSAR predictions in this case may not be reliable for the purpose of classification. In addition, acute toxicity data for mixtures of di- and tri- components in a ratio of 20:80 did not induce any fish mortality and algal EC_{50} values were above the respective water solubilities. Given the component is considered not readily biodegradable, is considered bioaccumulative, and has a water solubility below one mg/l, Chronic 4 may be applicable.

Commercial mixtures of styrenated phenol vary in composition of the mono-, di- and tri-components. Although representative compositions are employed in the risk assessment, industry should consider the composition of individual mixtures for CPL (GHS) classification. This is likely to need further consideration of available ecotoxicity data relevant to the mixture.

4.7 Assessment against PBT criteria

Characterisation of styrenated phenol as a PBT substance is currently incomplete. An assessment against the persistence, bioaccumulation and toxicity (PBT) criteria for the marine risk assessment is presented in Table 4.9.

Table 4.9 Screening classifications against PBT criteria.

Component	P, B or T	Information	Screening result	Refinement
Monostyrenated phenol	P	No specific data	not P or vP[2]	possible
	B	BCF_{fish} = 263[1]	not B	possible
	T	Lowest predicted NOEC 0.21 mg/l	not T	possible
Distyrenated phenol	P	No specific data	possible P/vP[2]	possible
	B	No accumulation	not B	-
	T	$NOEC_{Daphnia}$ = 0.115 mg/l Lowest predicted NOEC 0.045 mg/l for fish	not T	-
Tristyrenated phenol	P	No specific data	P or vP[2]	possible
	B	BCF_{fish} = 10,395[3]	vB for fish	not required
	T	No chronic effect on *Daphnia* at solubility. Lowest predicted NOEC 0.004 mg/l for fish	possible T	possible

[1] Calculated value from Table 3.15.

[2] Based on estimated values, see text.

[3] Growth-corrected value (non-growth corrected value is 6,695).

Persistence (P)

A substance is considered to be persistent (P) if it has a half-life over 60 days in marine water or over 40 days in fresh or estuarine water, or over 180 days in marine sediment or over 120 days in freshwater or estuarine sediment or soil. A substance is considered to be very persistent (vP) if it has a half-life over 60 days in marine, fresh or estuarine water, or over 180 days in marine, freshwater or estuarine sediment, or soil.

Information on the persistence of styrenated phenol is only available for the commercial product, which meets the screening criteria for 'P'. On this basis, styrenated phenol is not readily biodegradable and meets the persistence screening criteria. No simulation studies are available and the components are also hydrolytically stable

The BIOWIN program (USEPA, 2004) provides estimates of degradability and the results for the three styrenated phenol components are included in Appendix 2. The interpretation of the predictions set out in the Information Requirements for Chemical Safety Assessment, chapter 11 (ECHA, 2008b) uses three of the six values predicted, (in the combination BIOWIN 2 and BIOWIN 3 or BIOWIN 6 and BIOWIN 3), to indicate potential persistence – see Table 3.9 .

Monostyrenated phenol has only BIOWIN 6 below the threshold value and so does not meet the P criterion.

Distyrenated phenol also only has the BIOWIN 6 value below the threshold. However, the BIOWIN 3 value is within the range 2.2 to 2.7 which indicates uncertainty and further information is required to confirm if the substance is P or not.

Tristyrenated phenol has both BIOWIN 3 and BIOWIN 6 values below the relevant thresholds and so meets the P or vP screening criteria.

As tristyrenated phenol makes up 43 to 70 per cent of the commercial substance (in product A or B form), the overall prediction is that the substance meets the screening criteria as P or vP.

Further testing in simulation tests, focusing on the tristyrenated phenol component, would be possible to refine this part of the assessment.

Bioaccumulation (B)
A substance is considered to be bioaccumulative (B) if it has a bioconcentration factor (BCF) above 2,000 l/kg or very bioaccumulative (vB) if it has a BCF above 5,000 l/kg.

A fish-feeding bioaccumulation study indicates that tristyrenated phenol is accumulative, but that distyrenated phenol is not. A growth-corrected BCF value of 10,395 was calculated from the results of the fish feeding study with tristyrenated phenol, and this meets the vB criterion (the non-growth corrected value of 6,695 also meets the criterion). The monostyrenated component is predicted to be less bioaccumulative and does not exceed the threshold to be classified as ‘B’.

As tristyrenated phenol makes up over 40 per cent of the available commercial products, the overall conclusion is that styrenated phenol meets the B and vB criteria.

Although the Environment Agency does not consider that any more information is needed to make a decision on this end point, it is understood that some suppliers may be considering the practicalities of performing an OECD 305 BCF study, and a feasibility study is underway.

Toxicity (T)
A substance fulfils the toxicity criterion (T) when:

- the long-term no observed effect concentration (NOEC) for marine or freshwater organisms is less than 0.01 mg/l (10 µg/l);
- the substance is classified as carcinogenic (category 1 or 2), mutagenic (category 1 or 2) or toxic for reproduction (category 1, 2 or 3);
- there is other evidence of chronic toxicity, as identified by the classifications T, R48, or Xn, R48, according to Directive 67/548/EEC.

Styrenated phenol (as CAS number 61788-44-1 or 18254-13-2) is not listed in Directive 67/548/EEC.

The predicted NOEC values for the monostyrenated component are above the threshold value of 10 µg/l for the T criterion.

Distyrenated phenol has a measured NOEC for *Daphnia* above the T threshold. In addition, the lowest QSAR estimate (long-term fish NOEC 0.045 mg/l) is above the T threshold.

Tristyrenated phenol did not show effects at solubility in a chronic study with *Daphnia*. However, the QSAR estimate indicates fish may be more sensitive (see Section 4.1.8) and the predicted long-term fish NOEC is below the T threshold. The predicted values for fish and *Daphnia* are similar, and the available data for *Daphnia* suggests that the predictions may overestimate toxicity. While the measured values indicate that the substance is not T, the predicted fish NOEC is below the T criteria and further consideration may be required before a conclusion can be drawn on whether the substance meets the T criteria or not. A chronic fish toxicity test with tristyrenated phenol would allow this part of the assessment to be revised.

In addition, styrenated phenol does not meet the T criterion with respect to human health effects, although a full dataset is not yet available.

Overall
On the basis of the information available, styrenated phenol is categorised as persistent and very bioaccumulative in the environment, and may meet the vP and vB

criteria. Further assessment of the persistence of each component is recommended to allow some refinement of the conclusions. Priority should be given to simulation testing with the tristyrenated component, as the major component. It is not currently clear if styrenated phenol meets the T criteria given the predicted toxicity for tristyrenated phenol. A chronic toxicity study on fish with tristyrenated phenol would allow refinement against the T criteria but this is not recommended in the first instance as priority should be given to further P testing.

5 Risk characterisation

The following sections characterise risks for the aquatic, terrestrial and atmospheric compartments and the risk of secondary poisoning of predators in the food chain. The risk characterisation is performed by comparing PECs with PNECs to derive a risk characterisation ratio (RCR). An RCR below one implies that any risk resulting from that level of exposure is acceptable. An RCR above one implies a potential risk, and all such values are highlighted in bold in the following tables (RCRs are given to two significant figures).

For styrenated phenol, the risk characterisation is more complex than for simple substances in that there are three components to consider. As described in Section 1, this was addressed by calculating PEC values for the individual components, and comparing these with PNECs for the individual components. An overall ratio was calculated by summing the three separate ratios. This assumed that the effects are additive.

There were two exceptions to this approach, for wastewater treatment plants and for part of the secondary poisoning assessment. For these cases, PNECs were derived from results for the substance as a whole, and effectively assumed that each component in turn was responsible for all of the effects. This is a worst case approach, and summing the results in these cases is not considered to be reasonable.

The use areas listed in most of the following tables are defined in Section 3.3.

5.1 Aquatic compartment

5.1.1 Surface water

Risk characterisation ratios for surface water

The preliminary regional and local risk characterisation ratios for surface water are summarised in Table 5.1. Ratios for production are not presented; the emissions are considered to be negligible and hence there are no risks. The ‘Total’ figure given in each of the following tables is the sum of the individual RCRs.

Table 5.1 Local RCR values for surface water.

Use	$RCRlocal_{surface\ water}$			
	Monostyrenated phenol	**Distyrenated phenol**	**Tristyrenated phenol**	**Total**
Surfactant production	0.03	0.31	0.29	0.63
Surfactant formulation	<0.01	0.31	0.97	**1.3**
Agrochemical use	<0.01	0.019	0.31	0.33
Wool treatment	<0.01	0.30	0.94	**1.2**
Wool washing	<0.01	0.013	0.10	0.11
Rubber production	0.069	0.014	0.081	0.16
Rubber tyre production	<0.01	0.015	0.09	0.11
Rubber article production	<0.01	0.02	0.10	0.12
Regional	<0.01	0.012	0.08	0.092

The assessment shows risks for two of the scenarios, and only for the combined components. The main contribution to these risks comes from the tristyrenated component, and is based on an assumption of release in wastewater at the estimated solubility (7.1 µg/l) to surface water.

Section 4.1.8 includes alternative PNEC values for di- and tristyrenated phenol, derived from the ECOSAR program using the measured log K_{ow} values. Using these would add risks for surfactant production and for agrochemical use.

An alternative PNEC of 1.15 µg/l was derived in Section 4.1.8 from the only suitable experimental result available, relating to the distyrenated component. Comparing this value with the predicted concentrations of distyrenated phenol risks are indicated for surfactant production and formulation, and for wool treatment.

Uncertainties and possible refinements

There are uncertainties in the exposure and effects aspects of the assessment. Beginning with the estimates of emissions, for surfactant formulation these are based on default values from the TGD[23]. For wool treatment the estimates are based on industry-related information taken from an emission scenario document, but not on information specific to the substance. There is therefore scope for these estimates to be improved through more specific information on the processes involved and the behaviour of styrenated phenol during them. This could include information on waste treatment and disposal practices. In particular, the possible partitioning of the components within the process before discharge to water treatment (as for rubber production) could be important, especially as it is mainly the higher styrenated components which show a risk. Hence, more detailed information on the processes involved would be useful. Measurement of releases in wastewater or air may be necessary. The emission factors used were applied equally to all three components,

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[23] As noted in Section 3.1.3, information from a limited number of formulation sites indicates that emissions may be much lower.

though individual components may have different potentials for release. As far as possible, any measurements should be made for the three components individually.

The scenarios showing risk involve the release of styrenated phenol ethoxylates (as representatives for surfactants made with styrenated phenol) and include assumptions about the breakdown of ethoxylates and the amount of styrenated phenol regenerated. These assumptions are based on information for nonylphenol, and the behaviour of the styrenated phenol-based substances may be different. Testing on actual styrenated phenol-based surfactants, including the quantification of breakdown products, would allow more specific values to be used.

Information on the effects of styrenated phenol is limited, and predicted values were used in this assessment. There is some indication that predictions may overestimate toxicity, but further testing on other aquatic organisms would be needed to investigate this further. Testing on the tristyrenated component would be the most useful; however this would also be the most difficult in view of its low solubility. No effects were seen in a *Daphnia* study with tristyrenated phenol; hence testing on fish would be the next step if further toxicity testing were needed. Any such testing should await revision of the exposure scenarios.

5.1.2 Risk characterisation ratios for wastewater treatment plant microorganisms

The risk characterisation ratios for wastewater treatment plants are summarised in Table 5.2.

As described in Section 4.1.8 the PNEC for micro-organisms in wastewater treatment plants relates to a commercial product. To provide an initial assessment, as a worst case, it has been assumed that each component in turn is responsible for the toxicity. In this case the ratios are not combined.

Table 5.2 Local RCR values for wastewater treatment microorganisms.

Use	RCRlocal$_{wastewater}$		
	Monostyrenated phenol	**Distyrenated phenol**	**Tristyrenated phenol**
Surfactant production	0.063	0.037	<0.01
Surfactant formulation	<0.01	<0.01	<0.01
Agrochemical use	-	-	-
Wool treatment	<0.01	<0.01	<0.01
Wool washing	<0.01	<0.01	<0.01
Rubber production	0.14	<0.01	<0.01
Rubber tyre production	<0.01	<0.01	<0.01
Rubber article production	<0.01	<0.01	<0.01

There are no risks from any scenario.

The PNECs used above are the worst case values based on the data. An alternative (less conservative) approach is to compare the combined concentration of the three components with the PNEC values for the commercial product. The highest combined concentration for the three components in the wastewater treatment plant is 0.37 mg/l (see Table 3.3). The PNEC for the commercial product is 3.62 mg/l (Section 4.1.8). Hence there are no risks if this approach is employed.

5.1.3 Risk characterisation ratios for sediment

Risk characterisation ratios

The preliminary regional and local risk characterisation ratios for sediment are summarised in Table 5.3. RCRs of one or greater are highlighted in bold.

There are risks for all of the scenarios. In three cases the risk is only for the combined di- and tristyrenated components. For the other five scenarios, one or both of the di- and tristyrenated components gives rise to risks on its own. The ratios for di- and tristyrenated phenol are increased by a factor of ten to account for possible uptake through ingestion of the solid phase. Without this additional factor, the risks would be the same as those for the water compartment. There is also a risk for the regional sediment concentration[24], from the tristyrenated component, but only if the additional factor is applied.

Table 5.3 Local RCR values for sediment.

Use	$RCRlocal_{sediment}$			
	Monostyrenated phenol	**Distyrenated phenol**	**Tristyrenated phenol**	**Total**
Surfactant production[a]	0.03	**3.1**	**2.9**	**6.0**
Surfactant formulation	<0.01	**3.1**	**9.4**	**12.5**
Agrochemical use	<0.01	0.19	**3.1**	**3.3**
Wool treatment	<0.01	**3.0**	**9.4**	**12.4**
Wool washing	<0.01	0.13	1.0	**1.13**
Rubber production	0.068	0.14	0.81	**1.02**
Rubber tyre production	<0.01	0.15	0.91	**1.06**
Rubber article production	<0.01	0.19	**1.04**	**1.2**
Regional	<0.01	0.093	**1.6**	**1.8**

[a] The largest surfactant production site in the EU has negligible emissions and hence no risks.

Uncertainties and possible refinements

Improved information on emissions would refine the assessment for sediment. The emissions for surfactant production are based on default emission factors from the TGD, and should be capable of refinement[25]. Studies on the breakdown of surfactants would have an impact on the agrochemical use and wool washing scenarios. While such exposure information is needed for local scenarios for water, for sediment it may also help to refine the larger scale emissions and hence have an impact on the regional assessment (the regional contribution to local ratios for tristyrenated phenol is 0.9).

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[24] PECs for sediment are calculated from water PECs using the equilibrium partition approach. They are not calculated by adding the regional sediment concentration to the local contribution. Hence it is possible to have ratios below one for individual scenarios when the regional ratio is above one.

[25] Information from the main site producing styrenated phenol ethoxylates shows negligible emissions and no risks (Section 3.1.3).

The toxicity testing indicated for the aquatic compartment would also affect the sediment PNEC through equilibrium partitioning. However, the additional factor of ten applied for the di- and tristyrenated components means that such testing is unlikely to remove the risks on its own. Hence chronic testing on sediment organisms may be needed. This would probably require testing on two or three different species to obtain a significantly higher PNEC[26] (one test alone would require the use of an assessment factor of 100).

5.2 Terrestrial compartment

5.2.1 Risk characterisation ratios

The preliminary regional and local risk characterisation ratios for soil are summarised in Table 5.4. RCRs of one or greater are highlighted in bold.

Table 5.4 Local RCR values for soil.

Use	**$RCRlocal_{soil}$**			
	Monostyrenated phenol	**Distyrenated phenol**	**Tristyrenated phenol**	**Total**
Surfactant production	<0.01	<0.01	<0.01	<0.01
Surfactant formulation	0.11	**7.95**	**31**	**39**
Agrochemical use	<0.01	0.063	0.22	0.28
Wool treatment	0.10	**7.57**	**29**	**37**
Wool washing	<0.01	0.028	0.10	0.13
Rubber production	<0.01	<0.01	<0.01	<0.01
Rubber tyre production	<0.01	0.055	0.07	0.12
Rubber article production	<0.01	0.12	0.15	0.27
Regional	<0.01	0.12	**3.6**	**3.7**

An extra factor of 10 was applied to the RCRs for the distyrenated and tristyrenated components to allow for possible uptake through ingestion of soil-bound substances. This is a consequence of the log K_{ow} of these components being above five.

There are risks for two of the scenarios. In both of these the ratios would be above one without the additional factor; these have contributions from both di- and tristyrenated

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[26] An assessment factor of 100 would be applied to the result of one chronic sediment test. If the equilibrium partition method is correct, toxicity seen in the sediment test could be at about the level predicted from the lowest aquatic NOEC. In the equilibrium partition method, the lowest NOEC has a factor of 100 applied (10 for the NOEC and an additional 10 for the high log K_{ow}). The resulting PNECs could be roughly the same with only one sediment test, and further testing would be needed to give a higher PNEC for sediment. If uptake from the solid phase is also important, then the sediment NOEC could actually be lower than predicted by the equilibrium partition method.

phenol. There is also a risk for regional soil[27], only when the additional factor is applied and largely due to the tristyrenated component.

Uncertainties and possible refinements

The improved information on emissions and surfactant breakdown as described in Section 5.1.1 is also relevant here. In particular, information on the fate of sludge from wastewater treatment plants treating effluent from the relevant industries would be useful[28]. If this is applied to soil, measurement of the levels of the components in sludge would be useful, in particular for the di- and tristyrenated phenol.

The PNEC is derived using the equilibrium partition approach, so would be revised by any further aquatic toxicity testing. As for sediment, the additional factor of ten means that such testing may not remove the risks for soil. Again as for sediment, testing on two or three species may be needed to reach a significantly higher PNEC value. Both di- and tristyrenated phenols would need to be included. Again, this should wait for the outcome of the improved emission and concentration estimates.

5.3 Atmospheric compartment

Styrenated phenol is predicted to react rapidly with hydroxyl radicals in the atmosphere, although the products from such reactions are generally unknown. The very low volatilities of the main components of the mixture indicate that emissions to the environment are likely to be non-existent. As a consequence of the lack of relevant effects data, a PNEC for the atmospheric compartment was not calculated for styrenated phenol. However, in view of the low concentrations expected (all calculated to be less than 1×10^{-5} µg/m^3), risks are likely to be low.

5.4 Non-compartment specific effects relevant to the food chain (secondary poisoning)

5.4.1 Risk characterisation ratios

RCR values for secondary poisoning are summarised in Table 5.5 and Table 5.6. RCRs of one or greater are highlighted in bold. PNECs for secondary poisoning were developed as in Section 4.4.12. The ratios in Table 5.5 were derived from combined concentrations of the three components and the PNEC from commercial product A.

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[27] The regional risk characterisation for soil uses the concentration in agricultural soil in the regional model. The regional contribution to local PECs uses the concentration in natural soil, to avoid double-counting the substance applied to land. Hence the regional soil can show a risk when individual local scenarios do not.

[28] Information was provided by ETRMA for rubber scenarios – see Section 3.3.5.

Table 5.5 RCRs for secondary poisoning based on combined concentrations of components and PNEC of 11.11 mg/kg.

Use	Freshwater fish	Terrestrial	Marine predator	Marine top predator
Surfactant production	0.045	**4.7**	0.83	0.23
Surfactant formulation	0.15	**47**	0.015	<0.01
Agrochemical use	0.023	**5.0**	-	-
Wool treatment	0.12	**45**	0.013	<0.01
Wool washing	0.031	**4.8**	<0.01	<0.01
Rubber production	0.032	**4.7**	<0.01	<0.01
Tyre production	0.03	**4.8**	<0.01	<0.01
Article production	0.029	**4.9**	<0.01	<0.01

The ratios in Table 5.6 were derived using the concentrations of the individual components and the PNECs derived by assuming each component in turn was responsible for the toxicity. These are considered to be the worst case ratios.

Table 5.6 RCR values for secondary poisoning (using worst case PNECs for individual components).

Use	RCRs for aquatic food chain			RCRs for terrestrial food chain		
	Mono-	Di-	Tri-	Mono-	Di-	Tri-
Surfactant production	0.03	na	0.074	<0.01	0.11	**11**
Surfactant formulation	0.015	na	0.32	0.04	**7.1**	**103**
Agrochemical use	<0.01	na	0.045	<0.01	0.16	**11**
Wool treatment	0.011	na	0.25	0.04	**6.8**	**99**
Wool washing	<0.01	na	0.048	<0.01	0.13	**11**
Rubber production	0.03	na	0.042	<0.01	0.11	**11**
Rubber tyre production	<0.01	na	0.045	<0.01	0.16	**11**
Rubber article production	<0.01	na	0.044	<0.01	0.21	**11**

Mono, di and tri are monostyrenated, distyrenated and tristyrenated phenol respectively. [a] The largest surfactant production site in the EU has negligible emissions and hence no risks.

Both the ‘best case’ and ‘worst case’ PNEC values lead to no risks for the aquatic food chain but risks for all scenarios for the terrestrial food chain. In the worst case treatment for the terrestrial food chain, where the PNECs for di- and tristyrenated phenol are the same, the ratios for tristyrenated phenol are larger, and in some cases are the only ratios above one.

Uncertainties and possible refinements

Bioconcentration factors used in calculating the secondary poisoning exposures for the terrestrial food chain are estimated from the log K_{ow} values, and are very high for the di- and tristyrenated components. There are uncertainties in the predictions when using higher log K_{ow} values. It should be possible to combine the determination of worm BCFs with soil toxicity testing. The log K_{ow} value for the monostyrenated component is an estimated value and could be measured. As the measured log K_{ow} values for the other two components are higher than the estimated values, this could lead to an increase in the estimated BCF. However, the concentrations of this component are always small in comparison to the other two. It is not considered possible to read across from the fish accumulation studies to earthworms.

High accumulation and biomagnification factors for the soil food chain mean that the regional concentration in the secondary poisoning exposure derived from the regional soil concentrations is high enough to indicate risks without any contribution from local sources. In a number of scenarios, the local contribution is small and the risk is almost entirely due to the regional contribution. Therefore, refinement of the emissions on the regional (and continental) scale would have an impact on the secondary poisoning assessment. Some scenarios capable of improvement have already been identified in the preceding sections. The major contribution to the regional concentration comes from the degradation of ethoxylates used in agriculture. The assessment currently assumes complete degradation of the ethoxylates back to the parent substance; this could be investigated experimentally or in the field to determine a more realistic figure. Other sources such as tyre wear and wear from other rubber articles have only a small impact on the regional soil concentration (removing these emissions from the calculations has no effect on the risk ratios for the soil food chain).

The PNEC used in this assessment is based on exposure to a mixed product, and toxicity data for the individual components are not available. It would be possible to conduct tests on the components, of a longer duration so that a lower assessment factor could be used. Consideration of this should await the outcome of the revisions to the emissions and accumulation data.

5.5 Marine compartment

5.5.1 Risk characterisation ratios

RCRs for marine waters and sediment are summarised in Table 5.7. An extra factor of ten was applied to the RCRs for sediment for the distyrenated and tristyrenated components. This was to allow for possible uptake of the substance through ingestion of sediment-bound substances as a consequence of the log K_{ow} of these components being above five. Ratios for secondary poisoning in marine food chains are summarised in Table 5.5 (based on combined concentrations and the PNEC for the commercial product) and Table 5.8 (based on individual concentrations and PNECs for each component). In all tables, RCRs of one or greater are highlighted in bold.

The agrochemical use scenario is not considered relevant for the marine environment, and so no values were included for this scenario.

There are risks for three scenarios for the marine water assessment. The risk for surfactant production is increased by the use of a larger assessment factor (100) on the toxicity data and the assumption of direct release to marine waters without wastewater treatment, which together overcome the increased dilution used in the marine calculations. Two scenarios show risks only when the components are combined. The ratios for sediment are higher due to the additional factor applied to the di- and tristyrenated phenol as indicated above, and this leads to all scenarios showing a risk.

For the food chain exposure in the marine environment, one scenario shows a risk for marine predators when using the ‘worst case’ PNECs but not when using the ‘best case’ PNECs. No scenarios show risks for top predators using either approach.

Uncertainties and possible refinements

The same comments as above for the aquatic and secondary poisoning assessments are applicable here. A particular aspect for the marine assessment is whether there are direct discharges to marine waters (as is assumed for scenarios[29] in this assessment) rather than via wastewater treatment. Related to this is the more basic question of whether these activities have discharges to the marine environment. As noted in Section 3.3.5, the major surfactant producer in the EU does not discharge directly or indirectly to the marine environment. All of the wastewater from rubber production in Germany is treated before discharge, and the majority of tyre production sites in the EU do not have marine discharges. Hence, actual concentrations and risk ratios are expected to be lower in most cases. However, the presence of a wastewater treatment plant may not be sufficient to remove the possible concern. As an example, assuming the presence of a standard-size wastewater treatment plant for the rubber production scenario leads to ratios of 0.27, 0.19 and 1.13 for mono-, di- and tristyrenated phenol respectively, still indicating a risk.

It would be possible to refine the PNEC for marine waters by testing marine species, but the need for this should be decided after refinement of the exposure assessment.

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[29] The scenarios involving styrenated phenol ethoxylates include wastewater treatment plants before discharge to the marine environment, as it is this step which is assumed to lead to the formation of styrenated phenol through the breakdown of the ethoxylates.

Table 5.7 Local RCR values for the marine compartment.

Use	RCRlocal$_{\text{seawater}}$				RCRlocal$_{\text{marine sediment}}$			
	Monostyrenated phenol	**Distyrenated phenol**	**Tristyrenated phenol**	**Total**	**Monostyrenated phenol**	**Distyrenated phenol**	**Tristyrenated phenol**	**Total**
Surfactant production	0.14	**6.97**	**127**	**134**	0.14	**69.7**	**1,270**	**1,340**
Surfactant formulation	<0.01	0.31	0.97	**1.3**	<0.01	**3.1**	**9.7**	**13**
Agrochemical use	-	-	-	-	-	-	-	-
Wool treatment	<0.01	0.30	0.96	**1.3**	<0.01	**3.0**	**9.6**	**13**
Wool washing	<0.01	0.013	0.13	0.14	<0.01	0.13	**1.3**	**1.4**
Rubber production	0.33	0.054	0.14	0.52	0.33	0.54	**1.4**	**2.3**
Tyre production	<0.01	0.032	0.23	0.26	<0.01	0.32	**2.3**	**2.6**
Article production	<0.01	0.055	0.37	0.43	<0.01	0.55	**3.7**	**4.3**
Regional	<0.01	0.012	0.11	0.12	<0.01	0.23	**2.2**	**2.4**

Table 5.8 RCRs for food chain exposure in the marine environment.

Use	RCRlocal$_{marine\_predator}$			RCRlocal$_{marine\_top\ predator}$		
	Monostyrenated phenol	**Distyrenated phenol**	**Tristyrenated phenol**	**Monostyrenated phenol**	**Distyrenated phenol**	**Tristyrenated phenol**
Surfactant production	0.013	na	**1.93**	<0.01	na	0.52
Surfactant formulation	<0.01	na	0.036	<0.01	na	0.015
Agrochemical use	-	-	-	-	-	-
Wool treatment	<0.01	na	0.029	<0.01	na	0.013
Wool washing	<0.01	na	<0.01	<0.01	na	<0.01
Rubber production	0.014	na	<0.01	<0.01	na	<0.01
Rubber tyre production	<0.01	na	0.013	<0.01	na	<0.01
Rubber article production	<0.01	na	0.011	<0.01	na	<0.01

6 Conclusions

Styrenated phenol is used as an intermediate in the production of ethoxylate surfactants. These are used mainly in the formulation of crop protection products, with minor uses as anti-static agents for wool and as stabilisers for polyurethane foams (and in emulsion polymerisation, which is not addressed in this assessment). Styrenated phenol is also used as an antioxidant for rubber, being added to the rubber emulsion after polymerisation to reduce degradation. The substance is produced in the EU by four companies and is a high production volume substance (over 1,000 tonnes per year). There is no production in the UK, but the uses are relevant for the UK.

The commercial substance consists of three components, mono-, di- and tristyrenated phenol. The assessment estimates concentrations of the individual components and compares these with PNEC values for the relevant component. For some compartments (water, sediment, soil) risk ratios for individual components are summed; for wastewater treatment risks are considered individually; for secondary poisoning both approaches are used.

No risks are expected for air or wastewater treatment plants for any stage of the life cycle. Potential risks for the remaining risk assessment protection goals are highlighted in Table 6.1 (the actual risk characterisation ratios may be found in Section 5).

There are no risks for production for any compartment. There are no risks for wool washing and rubber production for the water and soil compartments (both shows risks to the sediment compartment). All scenarios[30] except production show risks to freshwater and marine sediment. All scenarios have risks for secondary poisoning for the terrestrial food chain. There are no risks for the freshwater food chain and for marine top predators, and only surfactant production shows a risk for marine predators.

6.1 Uncertainties

Uncertainties in the available data and in estimated and extrapolated values are noted throughout the assessment and in the risk characterisation section and are summarised here.

Emissions – release estimates for most of the scenarios are based on information specific to industrial sectors (in the form of emission scenario documents), but in general no information on releases for styrenated phenol is included in the assessment, with the exception of production and rubber polymerisation. For ethoxylate production and formulation, estimates are based on TGD default values.

Vapour pressures are calculated, and have a high degree of uncertainty. The emission from rubber articles in use is based on the vapour pressure, and if the value were much higher then the emission estimates would increase. However, emissions to air only have a small influence on the concentrations in water, sediment and soil and so this uncertainty has little impact on the assessment.

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[30] Agrochemical use in not included in the marine scenarios

Table 6.1 Life-cycle stages that flag as potential risks in this assessment.

Use	Fresh-water	Sediment	Freshwater food chain	Soil	Terrestrial food chain	Marine water	Marine sediment	Marine predators	Marine top predator
Production									
Surfactant production		■			■	■	■	■	
Surfactant formulation	■	■		■	■	■	■		
Agrochemical use		■			■				
Wool treatment	■	■		■	■	■	■		
Wool washing		■			■		■		
Rubber production		■			■		■		
Rubber tyre production		■			■		■		
Rubber article production		■			■		■		
Regional		■		■	■		■		

The assessment assumes that particles of rubber lost from tyres and other rubber articles during their lifetime release all their content of styrenated phenol to the environment. It is likely that some of this is reacted before the release occurs, but there is no way to estimate this at the moment. Removing these emissions from the calculations to test their contribution reduces concentrations, particularly at the regional level. However, only two risk ratios for freshwater sediment and one for marine sediment are reduced to below one, and regional soil and sediment ratios are still above one.

The indirect emission of styrenated phenol from the degradation of styrenated phenol ethoxylates is based on data for nonylphenol and octylphenol. Hence there is uncertainty in applying the values to the styrenated phenol ethoxylates.

Persistence – There is limited information on the persistence and half-lives of styrenated phenol in the environment. This has some influence on the assessment, but not in all areas. For example, the half-life of a substance in the environment (unless very short) has little effect on the local concentrations for water and sediment. This does not include the degree of degradation during wastewater treatment, which is assumed to be zero based on the available standard tests. Regional concentrations are likely to be influenced to a greater extent by the half-lives in the environment, and therefore better information on these could affect the assessment as risks are indicated for sediment and soil at the regional level. As an indication, the reaction of phenols with oxidants in water is discussed in Section 3.2.2 and a half-life of around 13 days is suggested. If this half-life is included in the calculations, the regional concentrations in sediment and marine sediments both decrease to below the relevant PNEC values. Such information is potentially relevant to the PBT assessment.

Physico-chemical properties – The log K_{ow} for monostyrenated phenol is estimated. Estimates for di- and tristyrenated phenol are lower than measured values, and so there is uncertainty over the monostyrenated value and over the other property values (including the bioconcentration factor) derived from it. However, the risk ratios for monostyrenated phenol are low.

The effect of uncertainty in the vapour pressure values on emissions is discussed above. The vapour pressure (through its use in calculating the Henry's Law constant) has an influence on the distribution of the substance. Changing the values by an order of magnitude has no significant impact on the distribution in wastewater treatment plants, or in the general environment.

Effects – There are only two measured aquatic toxicity values. Predicted long-term toxicity values were used to derive PNEC values for each component; these have a degree of uncertainty, which is expected to be greater for predictions based on higher log K_{ow} values (hence for the di- and tristyrenated phenols). Comparisons between measured and calculated values are limited, but suggest that predictions may overestimate the toxicity. Using the measured value alone leads to a lower PNEC and risks for more scenarios. For sediment and soil there was no specific data, and so the equilibrium partitioning method was used; as the di- and tristyrenated components have log K_{ow} values above five, an additional factor of ten was applied to the ratios, and this also adds uncertainty since the potential for uptake in sorbed form from the sediment and soil is unknown. There were no marine toxicity data, so the freshwater data set was used, which means the use of a larger assessment factor and an additional contribution to the uncertainty. There are limited data on endocrine disruption.

6.2 Refinements

Further information and testing which could improve the assessment are described in the risk characterisation. The main points from these can be summarised as follows.

PBT – Identification of a substance as a PBT or vPvB could have serious consequences for a substance, as the presumption for risk management would be a cessation of emissions. Therefore, further investigation of these aspects should be a priority. Persistence could be further investigated through simulation testing. The most relevant media for the di-and tristyrenated components would be sediment and soil, as these are where most of the substance is expected to be found. Testing in these two media would also be of relevance for the conventional risk assessment. There are indications that photo-initiated oxidation could be significant in water, and further investigation of this (through modelling or experiments) could have an impact on the conventional risk assessment. However, this is not the most relevant compartment for the assessment of persistence.

Mono- and distyrenated phenol do not meet the B criterion (based on log K_{ow} and experimental results respectively); tristyrenated phenol meets the vB criterion based on a fish feeding BCF study. It is unlikely these conclusions would be altered by further testing.

Neither mono- nor distyrenated phenol are considered T. It is currently unclear whether the tristyrenated component meets the T criteria. Additional toxicity testing, such as a chronic toxicity to fish study for the tristyrenated component, would aid refinement. Overall, this means it is not clear if styrenated phenol meets the T criteria. Further toxicity testing should await further assessment of persistence.

Releases - More specific information on possible releases from all areas of use. Direct measurement of emissions from processes would provide better estimates of releases. As far as possible these should measure the major components individually. Alternatively, demonstration that the process used does not lead to the release of styrenated phenol may be possible, as has been done for production. Where possible, information about the potential for releases to the marine environment and on the application of sludges to soils from specific industries would be useful (although for the more disperse uses, it may not be possible to collect sufficient information to override the current approaches).

Testing on the degradation of styrenated phenol-based surfactants, including the quantification of breakdown products, would allow more specific values to be used and the scenarios of ethoxylate use to be refined (as well as the contribution to the overall emissions from this source) Information on the physico-chemical poperties of the surfactants would also be useful in modelling their distribution.

Investigation into the release of styrenated phenol from abraded rubber particles from tyres and other rubber products would allow the estimates of releases from these sources to be refined, although the effect of this on assessment results may be limited.

Effects – If further long-term testing on aquatic organisms is indicated by the assessment, fish testing would be the next step.

For the sediment and terrestrial compartments, there is in principle a testing requirement for di- and tristyrenated phenol, and three chronic studies in both compartments could be required. The tests should ensure that the exposure concentrations cover the maximum predicted concentrations. Testing on freshwater organisms (water and sediment) would also help to refine the marine risk assessment, but testing may be required using marine organisms.

The PNEC for secondary poisoining could in principle be refined through chronic testing.

Consideration could be given to further investigation of endocrine disruption, where the data are currently limited. A review of results for substances of similar structure could provide indications of potential effects and of suitable species and methods for testing.

Any additional testing on effects should await the results of improved emission information gathering.

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List of abbreviations

Acronym	Description
ACC	American Chemistry Council
B	Bioaccumulative
BCF	Bioconcentration factor
BHT	2,6-Di-*tert*-butyl-*p*-cresol
BMF	Biomagnification factor
BTMA	British Tyre Manufacturers Association
bw	Body weight
CAS	Chemical Abstract Services
CEPAD	European Council for Alkylphenols and Derivatives
ChV	Chronic toxicity value
CoE	Council of Europe
CoMFA	Comparative Molecular Field Analysis
CoREPA	Common reactivity pattern approach
CPA	Crop Protection Agency
CSF	Chemical Stakeholder Forum
DEHP	Diethylhexyl phthalate
Defra	Department for Environment, Food and Rural Affairs
DSP	Distyrenated phenol
EA	Environment Agency
EC	European Commission
EC_x	As EC_{50}, but for x per cent effect; x usually being 0, 10, or 100
ECB	European Chemicals Bureau
ECHA	European Chemicals Agency
EINECS	European Inventory of Existing Commercial Chemical Substances – this lists all chemical substances supplied to the market prior to 18 September 1981
EPIWIN	Estimation Programs Interface Suite™
E-SBR	Styrene-butadiene rubber manufactured by emulsion polymerisation
ESD	Emission Scenario Document
ESIS	European chemical Substances Information System
ESR	Existing Substances Regulation – Council Regulation (EEC) 793/93 on the evaluation and control of risks of ‘existing’ substances
Etrma	European Tyre and Rubber Manufacturers Association
EU	European Union
EUSES	European Union System for the Evaluation of Substances (software tool in support of

Acronym	Description
	the TGD on risk assessment)
FEICA	Association of European Adhesives Manufacturers
GC	Gas chromatography/chromatogram
GLP	Good laboratory practice
HPLC	High pressure liquid chromatography
HPV	High production volume (supply over 1,000 tonnes/year)
HPVC	High production volume chemical (supply over 1,000 tonnes/year)
IUCLID	International Uniform Chemical Information Database: contains data collected under the Existing Substances Regulation (ESR)
K_{oc}	Organic carbon normalised distribution coefficient
K_{ow}	Octanol water partition coefficient
K_p	Solids-water partition coefficient
$L(E)C_{50}$	Median lethal (effect) concentration
LD_{50}	Median lethal dose
LOAEL	Lowest observed adverse effect level
LOEC	Lowest observed effect concentration
log K_{ow}	Log of the octanol-water partition coefficient (K_{ow})
LPVC	Low production volume chemical (supply 10-1,000 tonnes/year)
MBT	2-Mercaptobenzothiazole
MBTS	Benzothiazyl disulfide
MSP	Monostyrenated phenol
MTBE	Methyl tertiary butyl ether
NOAEL	No observed adverse effect level
NOEC	No observed effect concentration
n.t.p.	Normal temperature and pressure
OECD	Organisation for Economic Cooperation and Development
P	Persistent
PBT	Persistent, bioaccumulative and toxic
PCA	Paper Chemicals Association
PEC	Predicted environmental concentration
pKa	Logarithm (to the base 10) of the acid dissociation constant
PNEC	Predicted no-effect concentration
ppm	Parts per million
PU	Polyurethane
QSAR	Quantitative Structure-Activity Relationship
RCR	Risk characterisation ratio
REACH	Registration, Evaluation, Authorisation and

Acronym	Description
	Restriction of Chemicals
RN	Registry number
RR	Recovery rate
SBR	Styrene-butadiene rubber
SMILES	Simplified Molecular Input Line Entry System – the SMILES code is a chemical notation system used to represent a molecular structure by a linear string of symbols; it is a simple way of entering chemical structural information into a computer program
SP	Styrenated phenol
SPE	Styrenated phenol ethoxylate
SPTF	Styrenated Phenol Task Force
T	Toxic
TCPP	Tris(2-chloro-1-methylethyl) phosphate
TGD	Technical Guidance Document
TSP	Tristyrenated phenol
US	United States (of America)
USEPA	Environmental Protection Agency, USA
UK	United Kingdom
UKCCRMP	United Kingdom Coordinated Chemicals Risk Management Programme
vB	Very bioaccumulative
vP	Very persistent
VP	Vapour pressure
vPvB	Very persistent and very bioaccumulative
WAF	Water accommodated fraction
WS	Water solubility
WSF	Water soluble fraction
wwt	Wet weight
WWTP	Wastewater treatment plant

Glossary

Term	Description
Biochemical oxygen demand (BOD)	A measure of degradation potential
Bioconcentration factor (BCF)	A measure of chemical uptake; the ratio between the concentration in an organism and the concentration in an environmental compartment (usually water)
CAS number (no.)	An identifying code number assigned to chemicals by the Chemical Abstract Services. The CAS number is a generally recognised identification reference for a chemical; it is possible that a substance can have more than one such number
Lowest observed effect concentration (LOEC)	The lowest concentration in a toxicity test that gives rise to adverse effects (relative to a control)
Median effective concentration (EC_{50})	The concentration in a toxicity test at which a particular effect is observed in half of the organisms exposed for a specified time
Median lethal concentration/dose (LC/D_{50})	The concentration in a toxicity test that can be expected to cause death in half of the organisms exposed for a specified time
No observed effect concentration (NOEC)	The highest concentration in a toxicity test that does not give rise to adverse effects (relative to a control)
Octanol-water partition coefficient (K_{ow})	This parameter gives an indication of the partitioning behaviour of a substance between water and lipid-containing materials such as cell membranes or organic matter in soils and sediments
Readily biodegradable	Rapid environmental degradation to carbon dioxide and water, and so on, as measured by laboratory screening tests involving micro-organisms

Appendix 1

Data collection and peer review process

This report was produced using publicly available data gathered and assessed by the contractor for the Environment Agency. Additional information, including some original study reports, was submitted voluntarily by industry.

The Environment Agency was keen to ensure that the data used in this report were as complete and accurate as possible. Original reports and literature articles for key studies were retrieved and assessed for reliability wherever possible.

The initial data review began in 2005. The scientific literature was last searched in 2007 using Chemical Abstracts through STN (as well as Google®). The search terms were the CAS number and partial chemical names.

Drafts of this report were circulated in 2006, 2007 and 2008 to key partners in UK and European industry for comment as well as to members of the UK and international chemical regulatory communities (including the Advisory Committee on Hazardous Substances in September 2008). All comments received were addressed in the final report where appropriate. A full list of consultees is given at the end of this appendix.

In addition, certain technical aspects of the report were peer-reviewed by an independent expert group set up by the Environment Agency for this purpose in autumn 2008. Again, this report addresses those comments. Their comments have not been published but are available on request.

LIST OF KEY ORGANISATIONS CONSULTED IN PREPARATION OF REPORT

Industrial organisations

Aquaspersion UK
Association of Plastic Manufacturers in Europe (APME)
British Association of Chemical Speciality (BACS)
British Adhesives and Sealants Association (BASA)
British Adhesives and Sealants
British Rubber Chemicals Association (BRMA)
British Tyre Manufacturers Association (BTMA)
Centre Européen des Agents de Surface et de leurs Intermédiaires (Detergents Chemistry Sector) (CESIO)
Cognis
Conseil Européen des Phénols Alkylés et Derivés (European Council for Alkylphenols and Derivatives) (CEPAD)
Confederation of Paper Industries (CPI)
Eliokem
European Light Stabilizers and Antioxidant Association (ELiSANA)
European Rubber Chemicals Association (ERCA)
European Synthetic Rubber Association (ESRA)
Association of European Adhesives Manufacturers (FEICA)
CIA Sector group for organic surfactants and intermediate products (GOSIP)
Institute of Synthetic Rubber Producers (IISRP)
Lanxess
Paper Chemicals Association (PCA)
Performance Textiles Association

Paper Industry Technical Association (PITA)
Plastics Europe
Rhodia
Styrenated Phenol Task Force (SPTF)

UK government bodies

Advisory Committee on Hazardous Substances (ACHS)
Crop Protection Agency (CPA)
Department for Environment, Food and Rural Affairs (Defra)
Health and Safety Executive (HSE)

US government bodies

United States Environment Protection Agency (USEPA)

European regulatory authorities

EU PBT Working Group

Appendix 2

QSAR results for physicochemical properties, and environmental fate and behaviour

QSAR results for the components of styrenated phenol as determined by the EPIWIN (v3.12) computer estimation software program and the OECD (Q)SAR toolbox (v1.1) are presented below.

A2.1 EPIWIN predictions

A2.1.1a o-Monostyrenated phenol

SMILES: **c1(O)c(C(C)c2ccccc2)cccc1**
CHEM: o-MSP
MOL FOR: $C_{14}H_{14}O_1$
MOL WT: 198.27

Physical Property Inputs:
Water Solubility (mg/l): ------
Vapour Pressure (mm Hg): ------
Henry's LC (atm-m^3/mol): ------
Log K_{ow} (octanol-water): ------
Boiling Point (°C): ------
Melting Point (°C): ------

Log Octanol-Water Partition Coefficient (SRC):
Log K_{ow} (KOWWIN v1.67 estimate) = 3.67

Boiling Pt, Melting Pt, Vapour Pressure Estimations (MPBPWIN v1.41):
Boiling Pt (°C): 319.83 (Adapted Stein & Brown method)
Melting Pt (°C): 90.04 (Mean or Weighted MP)
VP(mm Hg, 25°C): 4.9×10^{-5} (Modified Grain method)

Water Solubility Estimate from Log K_{ow} (WSKOW v1.41):
Water Solubility at 25°C (mg/l): 124.7
Log K_{ow} used: 3.67 (estimated)
No-melting point equation used

Water Solubility Estimate from Fragments:
Water Solubility (v1.01 estimate) = 51.503 mg/l

ECOSAR Class Program (ECOSAR v0.99h):
Class(es) found: Phenols

Henry's Law Constant (25°C) [HENRYWIN v3.10]:
Bond Method: 6.63×10^{-8} atm-m^3/mol
Group Method: Incomplete
Henry's LC [VP/WS estimate using EPI values]: 1.025×10^{-7} atm-m^3/mol

Probability of Rapid Biodegradation (BIOWIN v4.02):
Biowin1 (Linear Model): 0.9517
Biowin2 (Non-Linear Model): 0.9701
Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 2.7646 (weeks)
Biowin4 (Primary Survey Model): 3.5377 (days-weeks)
Readily Biodegradable Probability (MITI Model):
Biowin5 (MITI Linear Model): 0.2511
Biowin6 (MITI Non-Linear Model): 0.2064
Ready Biodegradability Prediction: NO

Atmospheric Oxidation (25°C) [AopWin v1.91]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 46.9784×10^{-12} cm^3/molecule-sec
Half-Life = 0.228 Days (12-hour day; 1.5×10^6 OH/cm^3)
Half-Life = 2.732 Hours

Ozone Reaction:
No Ozone Reaction Estimation
Reaction With Nitrate Radicals May Be Important!

Soil Adsorption Coefficient (PCKOCWIN v1.66):
K_{oc}: 3.151×10^4
Log K_{oc}: 4.498

Aqueous Base/Acid-Catalyzed Hydrolysis (25°C) [HYDROWIN v1.67]:
Rate constants can NOT be estimated for this structure!

BCF Estimate from Log K_{ow} (BCFWIN v2.15):
Log BCF = 2.126 (BCF = 133.6)
Log K_{ow} used: 3.67 (estimated)

Volatilization from Water:
Henry LC: 6.63×10^{-8} atm-m^3/mol (estimated by Bond SAR Method)
Half-Life from Model River: 1.244×10^4 hours (518.2 days)
Half-Life from Model Lake: 1.358×10^5 hours (5,658 days)

Removal in Wastewater Treatment:
Total removal: 17.52 per cent
Total biodegradation: 0.22 per cent
Total sludge adsorption: 17.29 per cent
Total to air: 0.00 percent
(using 10,000 hour Bio P, A, S)

Removal in Wastewater Treatment:
Total removal: 91.02 per cent
Total biodegradation: 81.73 per cent
Total sludge adsorption: 9.30 per cent
Total to air: 0.00 per cent
(using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (per cent)	Half-Life (hour)	Emissions (kg/hour)
Air	0.352	5.46	1,000
Water	21.7	360	1,000
Soil	76.6	720	1,000
Sediment	1.37	3.24×10^3	0

Persistence Time: 539 hours

A2.1.1b p-Monostyrenated phenol

SMILES: **c1cc(O)ccc1C(C)c2ccccc2**
CHEM: p-MSP
MOL FOR: $C_{14}H_{14}O$
MOL WT: 198.27

Physical Property Inputs:
Water Solubility (mg/l): ------
Vapor Pressure (mm Hg): ------
Henry LC (atm-m^3/mol): ------
Log K_{ow} (octanol-water): ------
Boiling Point (°C): ------
Melting Point (°C): ------

Log Octanol-Water Partition Coef (SRC):
Log K_{ow} (KOWWIN v1.67 estimate) = 3.67

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):
Boiling Pt (°C): 319.83 (Adapted Stein & Brown method)
Melting Pt (°C): 90.04 (Mean or Weighted MP)
VP(mm Hg, 25°C): 4.9×10^{-5} (Modified Grain method)

Water Solubility Estimate from Log K_{ow} (WSKOW v1.41):
Water Solubility at 25 deg C (mg/l): 124.7
Log K_{ow} used: 3.67 (estimated)
No-melting point equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 51.503 mg/l

ECOSAR Class Program (ECOSAR v0.99h):
Class(es) found:
Phenols

Henry's Law Constant (25°C) [HENRYWIN v3.10]:
Bond Method: 6.63×10^{-8} atm-m^3/mol
Group Method: Incomplete
Henrys LC [VP/WSol estimate using EPI values]: 1.025×10^{-7} atm-m^3/mol

Probability of Rapid Biodegradation (BIOWIN v4.02):
Biowin1 (Linear Model): 0.9517
Biowin2 (Non-Linear Model): 0.9701
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.7646 (weeks)
Biowin4 (Primary Survey Model): 3.5377 (days-weeks)
Readily Biodegradable Probability (MITI Model):
Biowin5 (MITI Linear Model): 0.2511
Biowin6 (MITI Non-Linear Model): 0.2064
Ready Biodegradability Prediction: NO

Atmospheric Oxidation (25°C) [AopWin v1.91]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 46.9784×10^{-12} cm^3/molecule-sec
Half-Life = 0.228 Days (12-hour day; 1.5×10^6 OH/cm^3)
Half-Life = 2.732 Hours

Ozone Reaction:
No Ozone Reaction Estimation
Reaction With Nitrate Radicals May Be Important!

Soil Adsorption Coefficient (PCKOCWIN v1.66):
K_{oc}: 3.087×10^4
Log K_{oc}: 4.490

Aqueous Base/Acid-Catalyzed Hydrolysis (25°C) [HYDROWIN v1.67]:
Rate constants can NOT be estimated for this structure!

BCF Estimate from Log K_{ow} (BCFWIN v2.15):
Log BCF = 2.126 (BCF = 133.6)
Log K_{ow} used: 3.67 (estimated)

Volatilization from Water:
Henry LC: 6.63E-008 atm-m^3/mol (estimated by Bond SAR Method)
Half-Life from Model River: 1.244×10^4 hours (518.2 days)
Half-Life from Model Lake: 1.358×10^5 hours (5,658 days)

Removal in Wastewater Treatment:
Total removal: 17.52 per cent
Total biodegradation: 0.22 per cent
Total sludge adsorption: 17.29 per cent
Total to air: 0.00 per cent
(using 10,000 hour Bio P, A, S)

Removal in Wastewater Treatment:
Total removal: 91.02 per cent
Total biodegradation: 81.73 per cent
Total sludge adsorption: 9.30 per cent
Total to air: 0.00 per cent
(using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (per cent)	Half-Life (hour)	Emissions (kg/hour)
Air	0.352	5.46	1,000
Water	21.7	360	1,000
Soil	76.6	720	1,000
Sediment	1.37	3.24×10^3	0

Persistence Time: 539 hours

A2.1.2a 2,4-Distyrenated phenol

SMILES: **c1(O)c(C(C)c2ccccc2)cc(C(C)c3ccccc3)cc1**
CHEM: 2,4-DSP
MOL FOR: $C_{22}H_{22}O$
MOL WT: 302.42

Physical Property Inputs:

Water Solubility (mg/l):	------
Vapour Pressure (mm Hg):	------
Henry's LC (atm-m^3/mol):	------

Log K_{ow} (octanol-water): ------
Boiling Point (°C): ------
Melting Point (°C): ------

Log Octanol-Water Partition Coefficient (SRC):
Log K_{ow} (KOWWIN v1.67 estimate) = 5.83

Boiling Pt, Melting Pt, Vapour Pressure Estimations (MPBPWIN v1.41):
Boiling Pt (°C): 422.06 (Adapted Stein & Brown method)
Melting Pt (°C): 159.09 (Mean or Weighted MP)
VP (mm Hg, 25°C): 1.93×10^{-8} (Modified Grain method)

Water Solubility Estimate from Log K_{ow} (WSKOW v1.41):
Water Solubility at 25°C (mg/l): 0.4776
Log K_{ow} used: 5.83 (estimated)
No-melting point equation used

Water Solubility Estimate from Fragments:
Water Solubility (v1.01 est) = 0.041883 mg/l

ECOSAR Class Program (ECOSAR v0.99h):
Class(es) found: Phenols

Henry's Law Constant (25 °C) [HENRYWIN v3.10]:
Bond Method: 7.84×10^{-9} atm-m^3/mol
Group Method: Incomplete
Henrys LC [VP/WS estimate using EPI values]: 1.608×10^{-8} atm-m^3/mol

Probability of Rapid Biodegradation (BIOWIN v4.02):
Biowin1 (Linear Model): 1.0849
Biowin2 (Non-Linear Model): 0.9876
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.4816 (weeks-months)
Biowin4 (Primary Survey Model): 3.3238 (days-weeks)
Readily Biodegradable Probability (MITI Model):
Biowin5 (MITI Linear Model): -0.0352
Biowin6 (MITI Non-Linear Model): 0.0268
Ready Biodegradability Prediction: NO

Atmospheric Oxidation (25°C) [AopWin v1.91]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 61.8678×10^{-12} cm^3/molecule-sec
Half-Life = 0.173 Days (12-hr day; 1.5×10^{-6} OH/cm^3)
Half-Life = 2.075 Hours

Ozone Reaction:
No Ozone Reaction Estimation
Reaction With Nitrate Radicals May Be Important!

Soil Adsorption Coefficient (PCKOCWIN v1.66):
K_{oc}: 3.63×10^{6}
Log K_{oc}: 6.560

Aqueous Base/Acid-Catalyzed Hydrolysis (25°C) [HYDROWIN v1.67]:
Rate constants can NOT be estimated for this structure!

BCF Estimate from Log K_{ow} (BCFWIN v2.15):
Log BCF = 3.786 (BCF = 6,116)
Log K_{ow} used: 5.83 (estimated)

Volatilization from Water:

Henry's LC: 7.84×10^{-9} atm-m^3/mol (estimated by Bond SAR Method)
Half-Life from Model River: 1.299×10^5 hours (5,411 days)
Half-Life from Model Lake: 1.417×10^6 hours (5.904×10^4 days)

Removal in Wastewater Treatment:
Total removal: 91.27 per cent
Total biodegradation: 0.76 per cent
Total sludge adsorption: 90.51 per cent
Total to air: 0.00 per cent
(using 10,000 hour Bio P, A, S)

Removal in Wastewater Treatment:
Total removal: 98.55 per cent
Total biodegradation: 38.37 per cent
Total sludge adsorption: 60.19 per cent
Total to air: 0.00 per cent
(using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (per cent)	Half-Life (hour)	Emission (kg/hour)
Air	0.0428	4.15	1,000
Water	4.44	900	1,000
Soil	44.9	1.8×10^3	1,000
Sediment	50.7	8.1×10^3	0

Persistence Time: 2.63×10^3 hours

A2.1.2b 2,6-Distyrenated phenol

SMILES : c1(C(C)c3ccccc3)c(O)c(C(C)c2ccccc2)ccc1
CHEM: 2,6-DSP
MOL FOR: $C_{22}H_{22}O$
MOL WT: 302.42

Physical Property Inputs:

Water Solubility (mg/l):	------
Vapor Pressure (mm Hg):	------
Henry's LC (atm-m^3/mol):	------
Log K_{ow} (octanol-water):	------
Boiling Point (°C):	------
Melting Point (°C):	------

Log Octanol-Water Partition Coef (SRC):
Log K_{ow} (KOWWIN v1.67 estimate) = 4.98

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):
Boiling Pt (°C): 422.06 (Adapted Stein & Brown method)
Melting Pt (°C): 159.09 (Mean or Weighted MP)
VP(mm Hg, 25°C): 1.93×10^{-8} (Modified Grain method)

Water Solubility Estimate from Log K_{ow} (WSKOW v1.41):
Water Solubility at 25°C (mg/l): 2.541
Log K_{ow} used: 4.98 (estimated)
No-melting point equation used

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 0.041883 mg/l

ECOSAR Class Program (ECOSAR v0.99h):
Class(es) found: Phenols

Henry's Law Constant (25°C) [HENRYWIN v3.10]:
Bond Method: 7.84×10^{-9} atm-m^3/mol
Group Method: Incomplete
Henry's LC [VP/WSol estimate using EPI values]: 3.022×10^{-9} atm-m^3/mol

Probability of Rapid Biodegradation (BIOWIN v4.02):
Biowin1 (Linear Model): 1.0849
Biowin2 (Non-Linear Model): 0.9876
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.4816 (weeks-months)
Biowin4 (Primary Survey Model): 3.3238 (days-weeks)
Readily Biodegradable Probability (MITI Model):
Biowin5 (MITI Linear Model): -0.0352
Biowin6 (MITI Non-Linear Model): 0.0268
Ready Biodegradability Prediction: NO

Atmospheric Oxidation (25°C) [AopWin v1.91]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 61.8678×10^{-12} cm^3/molecule-sec
Half-Life = 0.173 Days (12-hour day; 1.5×10^6 OH/cm^3)
Half-Life = 2.075 Hours

Ozone Reaction:
No Ozone Reaction Estimation
Reaction With Nitrate Radicals May Be Important!

Soil Adsorption Coefficient (PCKOCWIN v1.66):
K_{oc} : 3.705×10^6
Log K_{oc}: 6.569

Aqueous Base/Acid-Catalyzed Hydrolysis (25°C) [HYDROWIN v1.67]:
Rate constants can NOT be estimated for this structure!

BCF Estimate from Log K_{ow} (BCFWIN v2.15):
Log BCF = 3.132 (BCF = 1,355)
Log K_{ow} used: 4.98 (estimated)

Volatilization from Water:
Henry's LC: 7.84×10^{-9} atm-m^3/mol (estimated by Bond SAR Method)
Half-Life from Model River: 1.299×10^5 hours (5,411 days)
Half-Life from Model Lake: 1.417×10^6 hours (5.904×10^4 days)

Removal in Wastewater Treatment:
Total removal: 77.06 per cent
Total biodegradation: 0.67 per cent
Total sludge adsorption: 76.38 per cent
Total to air: 0.00 per cent
(using 10,000 hour Bio P, A, S)

Removal in Wastewater Treatment:
Total removal: 95.01 per cent

Total biodegradation: 43.29 per cent
Total sludge adsorption: 51.72 per cent
Total to air: 0.00 percent
(using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (per cent)	Half-Life (hour)	Emissions (kg/hour)
Air	0.0649	4.15	1,000
Water	10	900	1,000
Soil	68	1.8×10^3	1,000
Sediment	21.9	8.1×10^3	0

Persistence Time: 1.73×10^3 hour

A2.1.3 Tristyrenated phenol

SMILES: c(ccc1C(c(cc(c2O)C(c(ccc3)cc3)C)cc2C(c(ccc4)cc4)C)C)cc1
CHEM: TSP
MOL FOR: $C_{30}H_{30}O$
MOL WT: 406.57

Physical Property Inputs:
Water Solubility (mg/l): ------
Vapor Pressure (mm Hg): ------
Henry's LC (atm-m^3/mol): ------
Log K_{ow} (octanol-water): ------
Boiling Point (°C): ------
Melting Point (°C): ------

Log Octanol-Water Partition Coef (SRC):
Log K_{ow} (KOWWIN v1.67 estimate) = 7.13

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):
Boiling Pt (°C): 522.42 (Adapted Stein & Brown method)
Melting Pt (°C): 223.07 (Mean or Weighted MP)
VP(mm Hg, 25°C): 6.52E-012 (Modified Grain method)

Water Solubility Estimate from Log K_{ow} (WSKOW v1.41):
Water Solubility at 25°C (mg/l): 0.008576
Log K_{ow} used: 7.13 (estimated)
No-melting point equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 3.002×10^{-5} mg/l

ECOSAR Class Program (ECOSAR v0.99h):
Class(es) found: Phenols

Henry's Law Constant (25°C) [HENRYWIN v3.10]:
Bond Method: 9.27×10^{-10} atm-m^3/mol
Group Method: Incomplete
Henry's LC [VP/WSol estimate using EPI values]: 4.067×10^{-10} atm-m^3/mol

Probability of Rapid Biodegradation (BIOWIN v4.02):
Biowin1 (Linear Model): 1.2181

Biowin2 (Non-Linear Model): 0.9949
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.1986 (months)
Biowin4 (Primary Survey Model): 3.1099 (weeks)
Readily Biodegradable Probability (MITI Model):
Biowin5 (MITI Linear Model): -0.3215
Biowin6 (MITI Non-Linear Model): 0.0029
Ready Biodegradability Prediction: NO

Atmospheric Oxidation (25°C) [AopWin v1.91]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 38.2647×10^{-12} cm^3/molecule-sec
Half-Life = 0.280 Days (12-hour day; 1.5×10^6 OH/cm^3)
Half-Life = 3.354 Hours

Ozone Reaction: No Ozone Reaction Estimation
Reaction With Nitrate Radicals May Be Important!

Soil Adsorption Coefficient (PCKOCWIN v1.66):
K_{oc}: 4.268×10^8
Log K_{oc}: 8.630

Aqueous Base/Acid-Catalyzed Hydrolysis (25°C) [HYDROWIN v1.67]:
Rate constants can NOT be estimated for this structure!

BCF Estimate from Log K_{ow} (BCFWIN v2.15):
Log BCF = 4.627 (BCF = 4.237×10^4)
Log K_{ow} used: 7.13 (estimated)

Volatilization from Water:
Henry's LC: 9.27×10^{-10} atm-m^3/mol (estimated by Bond SAR Method)
Half-Life from Model River: 1.274×10^6 hours (5.306×10^4 days)
Half-Life from Model Lake: 1.389×10^7 hours (5.789×10^5 days)

Removal in Wastewater Treatment:
Total removal: 93.89 per cent
Total biodegradation: 0.78 per cent
Total sludge adsorption: 93.12 per cent
Total to air: 0.00 per cent
(using 10,000 hour Bio P, A, S)

Removal in Wastewater Treatment:
Total removal: 97.59 per cent
Total biodegradation: 25.58 per cent
Total sludge adsorption: 72.01 per cent
Total to air: 0.00 per cent
(using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (per cent)	Half-Life (hour)	Emissions (kg/hour)
Air	0.0467	6.71	1,000
Water	1.46	1.44×10^3	1,000
Soil	33.7	2.88×10^3	1,000
Sediment	64.8	1.3×10^4	0

Persistence Time: 4.92×10^3 hour

A2.1.4 TSPE028

This structure has been used to represent styrenated phenol ethoxylates.

SMILES:
OCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOc1c(C(C)c2ccccc2)cc(C(C)c3ccccc3)cc1C(C)c4ccccc4
CHEM: TSP28EO
MOL FOR: $C_{86}H_{142}O_{29}$
MOL WT: 1640.07

Physical Property Inputs:

Water Solubility (mg/l):	------
Vapor Pressure (mm Hg):	------
Henry's LC (atm-m^3/mol):	------
Log K_{ow} (octanol-water):	------
Boiling Point (°C):	------
Melting Point (°C):	------

Log Octanol-Water Partition Coef (SRC):
Log K_{ow} (KOWWIN v1.67 estimate) = 0.16

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):
Boiling Pt (°C): 1518.36 (Adapted Stein & Brown method)
Melting Pt (°C): 349.84 (Mean or Weighted MP)
VP(mm Hg, 25 °C): 0 (Modified Grain method)

Water Solubility Estimate from Log K_{ow} (WSKOW v1.41):
Water Solubility at 25°C (mg/l): 2.771e-005
Log K_{ow} used: 0.16 (estimated)
No-melting point equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 8.8496 mg/l

ECOSAR Class Program (ECOSAR v0.99h):
Class(es) found:
Surfactants-nonionic

Henry's Law Constant (25°C) [HENRYWIN v3.10]:
Bond Method: Incomplete
Group Method: Incomplete
Henry's LC [VP/WSol estimate using EPI values]: not available

Probability of Rapid Biodegradation (BIOWIN v4.02):
Biowin1 (Linear Model): -8.5731
Biowin2 (Non-Linear Model): 0.0000
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): -0.7159 (recalcitrant)
Biowin4 (Primary Survey Model): 1.2342 (recalcitrant)
Readily Biodegradable Probability (MITI Model):
Biowin5 (MITI Linear Model): -0.8920
Biowin6 (MITI Non-Linear Model): 0.0000
Ready Biodegradability Prediction: NO

Atmospheric Oxidation (25°C) [AopWin v1.91]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 440.9299×10-12 cm^3/molecule-sec
Half-Life = 0.024 Days (12-hour day; 1.5×10^6 OH/cm^3)
Half-Life = 17.466 Min
Ozone Reaction:
No Ozone Reaction Estimation

Soil Adsorption Coefficient (PCKOCWIN v1.66):
K_{oc}: 1×10^{10}
Log K_{oc}: 19.969

Aqueous Base/Acid-Catalyzed Hydrolysis (25°C) [HYDROWIN v1.67]:
Rate constants can NOT be estimated for this structure!

BCF Estimate from Log K_{ow} (BCFWIN v2.15):
Log BCF = 0.500 (BCF = 3.162)
Log K_{ow} used: 0.16 (estimated)

Volatilization from Water:
Henry's LC: 7.79×10^{-11} atm-m^3/mol (calculated from VP/WS)
Half-Life from Model River: 3.045×10^7 hours (1.269×10^6 days)
Half-Life from Model Lake: 3.321×10^8 hours (1.384×10^7 days)

Removal in Wastewater Treatment:

Total removal:	1.85 per cent
Total biodegradation:	0.09 per cent
Total sludge adsorption:	1.76 per cent
Total to air:	0.00 per cent

(using 10,000 hr Bio P, A, S)

Removal in Wastewater Treatment:

Total removal:	1.85 per cent
Total biodegradation:	0.09 per cent
Total sludge adsorption:	1.76 per cent
Total to air:	0.00 per cent

(using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (per cent)	Half-Life (hour)	Emissions (kg/hour)
Air	0.0287	0.582	1,000
Water	58.7	4.32×10^3	1,000
Soil	41.2	8.64×10^3	1,000
Sediment	0.117	3.89×10^4	0

Persistence Time: 945 hr

A2.2 OECD (Q)SAR toolbox

A2.2.1a o-Monostyrenated phenol

OECD Toolbox Application study history

Report created: 22.04.09 - 16:42

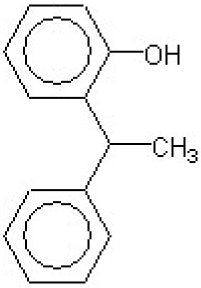
Chemical input *22.04.09 - 16:02*

Input single target chemical by: CAS number

CAS # :4237-44-9

Chemical name: Phenol, 2-(1-phenylethyl)-

SMILES: c1(O)c(C(C)c2ccccc2)cccc1



Profiling *22.04.09 - 16:03*

EcoSAR Classification

Phenols

ER-binding

Moderate binder, OH

Data gap filling *22.04.09 - 16:06*

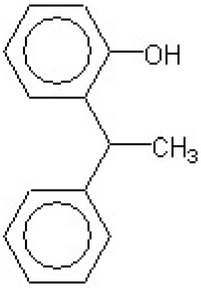
Entering data gap filling with: 0 datapoints

Filling GAP: LogP oct/water:

Target chemical

CAS# 4237-44-9

Chemical name: Phenol, 2-(1-phenylethyl)-



Entering data gap filling section:

Exiting data gap filling section:

Predicted value for "LogP oct/water:" was accepted,

Predicted "LogP oct/water:" = 4.45

Gaps filling approach = "QSAR"

Original QSAR model - "logP_Multicase"

Built - NO

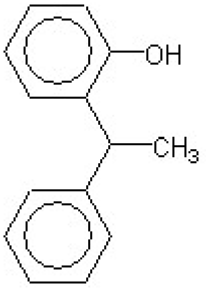
Entering data gap filling with: 0 datapoints

Filling GAP: Water Solubility

Target chemical

CAS# 4237-44-9

Chemical name: Phenol, 2-(1-phenylethyl)-



Entering data gap filling section:

Exiting data gap filling section:

Predicted value for "Water Solubility" was accepted,

Predicted "Water Solubility" = 37.0 mg/l

Gaps filling approach = "QSAR"

Original QSAR model - "WS_Multicase"

Built - NO

A2.2.1b p-Monostyrenated phenol

OECD Toolbox Application study history

Report created: 22.04.09 - 16:52

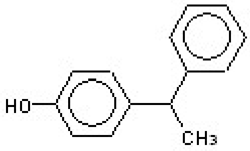
Chemical input *22.04.09 - 16:49*

Input single target chemical by: CAS number

CAS # :1988-89-2

Chemical name: Phenol, 4-(1-phenylethyl)-

SMILES: c1(C(C)c2ccc(O)cc2)ccccc1



Profiling *22.04.09 - 16:49*

EcoSAR Classification

Phenols

ER-binding

Moderate binder, OH

Data gap filling *22.04.09 - 16:51*

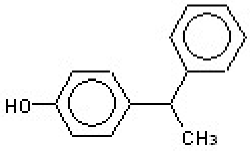
Entering data gap filling with: 0 datapoints

Filling GAP: Water Solubility

Target chemical

CAS# 1988-89-2

Chemical name: Phenol, 4-(1-phenylethyl)-



Entering data gap filling section:

Exiting data gap filling section:

Predicted value for "Water Solubility" was accepted,

Predicted "Water Solubility" = 88.0 mg/l

Gaps filling approach = "QSAR"

Original QSAR model - "WS_Multicase"

Built - NO

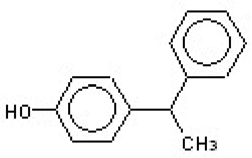
Entering data gap filling with: 0 datapoints

Filling GAP: LogP oct/water:

Target chemical

CAS# 1988-89-2

Chemical name: Phenol, 4-(1-phenylethyl)-



Entering data gap filling section:

Exiting data gap filling section:

Predicted value for "LogP oct/water:" was accepted,

Predicted "LogP oct/water:" = 4.38

Gaps filling approach = "QSAR"

Original QSAR model - "logP_Multicase"

Built – NO

A2.2.2a 2,4-Distyrenated phenol

OECD Toolbox Application study history

Report created: 22.04.09 - 16:55

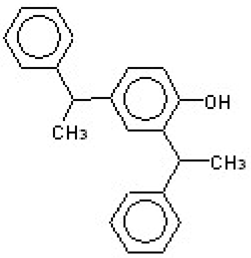
Chemical input *22.04.09 - 16:54*

Input single target chemical by: CAS number

CAS # :2769-94-0

Chemical name: Phenol, 2,4-bis(1-phenylethyl)-

SMILES: c1(O)c(C(C)c2ccccc2)cc(C(C)c2ccccc2)cc1



Profiling *22.04.09 - 16:54*

EcoSAR Classification

Phenols

ER-binding

Strong binder, OH

Data gap filling *22.04.09 - 16:55*

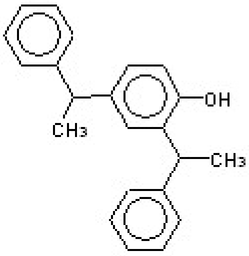
Entering data gap filling with: 0 datapoints

Filling GAP: Water Solubility

Target chemical

CAS# 2769-94-0

Chemical name: Phenol, 2,4-bis(1-phenylethyl)-



Entering data gap filling section:

Exiting data gap filling section:

Predicted value for "Water Solubility" was accepted,

Predicted "Water Solubility" = 0.0315 mg/l

Gaps filling approach = "QSAR"

Original QSAR model - "WS_Multicase"

Built - NO

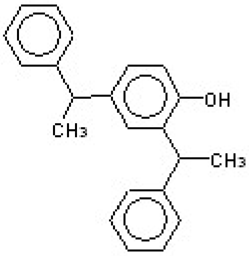
Entering data gap filling with: 0 datapoints

Filling GAP: LogP oct/water:

Target chemical

CAS# 2769-94-0

Chemical name: Phenol, 2,4-bis(1-phenylethyl)-



Entering data gap filling section:

Exiting data gap filling section:

Predicted value for "LogP oct/water:" was accepted,

Predicted "LogP oct/water:" = 7.03

Gaps filling approach = "QSAR"

Original QSAR model - "logP_Multicase"

Built – NO

A2.2.2b 2,6-Distyrenated phenol

OECD Toolbox Application study history

Report created: 22.04.09 - 16:59

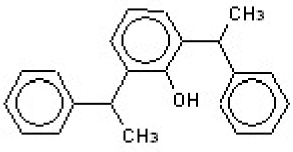
Chemical input *22.04.09 - 16:57*

Input single target chemical by: Drawing

CAS # :N/A

Chemical name:

SMILES: c1(C(C)c2ccccc2)c(O)c(C(C)c2ccccc2)ccc1



Profiling *22.04.09 - 16:57*

EcoSAR Classification

Phenols

ER-binding

With impaired OH or NH2 group

Data gap filling *22.04.09 - 16:59*

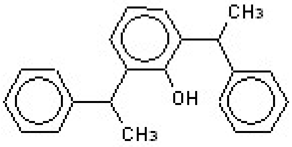
Entering data gap filling with: 0 datapoints

Filling GAP: Water Solubility

Target chemical

CAS# N/A

Chemical name:



Entering data gap filling section:

Exiting data gap filling section:

Predicted value for "Water Solubility" was accepted,

Predicted "Water Solubility" = 0.0228 mg/l

Gaps filling approach = "QSAR"

Original QSAR model - "WS_Multicase"

Built - NO

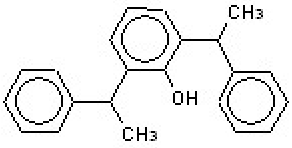
Entering data gap filling with: 0 datapoints

Filling GAP: LogP oct/water:

Target chemical

CAS# N/A

Chemical name:



Entering data gap filling section:

Exiting data gap filling section:

Predicted value for "LogP oct/water:" was accepted,

Predicted "LogP oct/water:" = 7.09

Gaps filling approach = "QSAR"

Original QSAR model - "logP_Multicase"

Built - NO

A2.2.3 Tristyrenated phenol

OECD Toolbox Application study history

Report created: 22.04.09 - 17:06

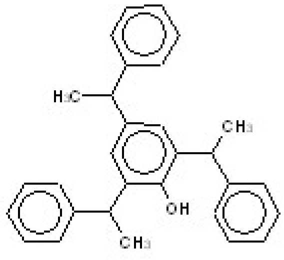
Chemical input *22.04.09 - 17:01*

Input single target chemical by: Drawing

CAS # :18254-13-2

Chemical name: Phenol, 2,4,6-tris(1-phenylethyl)-

SMILES: c1(C(C)c2ccccc2)c(O)c(C(C)c2ccccc2)cc(C(C)c2ccccc2)c1



Profiling *22.04.09 - 17:01*

EcoSAR Classification

Phenols

ER-binding

With impaired OH or NH2 group

Data gap filling *22.04.09 - 17:05*

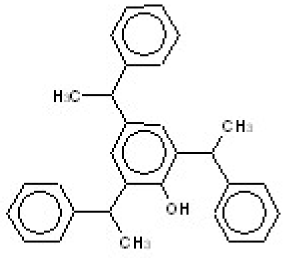
Entering data gap filling with: 0 datapoints

Filling GAP: Water Solubility

Target chemical

CAS# 18254-13-2

Chemical name: Phenol, 2,4,6-tris(1-phenylethyl)-



Entering data gap filling section:

Exiting data gap filling section:

Predicted value for "Water Solubility" was accepted,

Predicted "Water Solubility" = 3.04E-4 mg/l

Gaps filling approach = "QSAR"

Original QSAR model - "WS_Multicase"

Built - NO

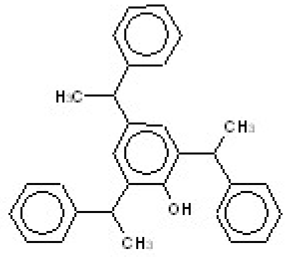
Entering data gap filling with: 0 datapoints

Filling GAP: LogP oct/water:

Target chemical

CAS# 18254-13-2

Chemical name: Phenol, 2,4,6-tris(1-phenylethyl)-



Entering data gap filling section:

Exiting data gap filling section:

Predicted value for "LogP oct/water:" was accepted,

Predicted "LogP oct/water:" = 9.63

Gaps filling approach = "QSAR"

Original QSAR model - "logP_Multicase"

Built - NO

QSAR Results for Toxicity Assessment

QSAR results for the components of styrenated phenol as determined by the ECOSAR program (v0.99h) are presented below. These use the estimated log K_{ow} values from EPIWIN (calculations using the measured log Kow values were not performed other than for distyrenated phenol, see Section 4.1.8).

The equations used in ECOSAR were developed with differing numbers of substances. The substances were mainly alkyl- and halogen-substituted phenols. The alkyl-substituted phenols included some multiply-substituted substances. There are no indications that the structures present in styrenated phenol do not fit into the group.

Warnings of possible excess toxicity over and above that predicted by the equations are given for 1,2- and 1,4-dihydroxy benzene and related substances.

The highest log K_{ow} value involved in the training data sets is 5.3 for most equations, the exceptions being acute fish (highest log K_{ow} 11) acute *Daphnia* (highest log K_{ow} 8) and 30-day fish (highest log K_{ow} 5.1). The equations suggest cut-off values of log K_{ow}; for the chronic equations, all three styrenated phenol components have values lower than the suggested cut-off.

It is concluded that the equations are appropriate for use with styrenated phenol, with the general proviso that estimates at high log K_{ow} values (those for di- and tristyrenated phenol) will be subject to greater uncertainty.

The following QSAR results were calculated using the log K_{ow} values predicted by EPIWIN. This reflects the QSAR methodology used to derive the predictive equations in ECOSAR. In addition, comparisons of QSAR predictions based on calculated log K_{ow} values were closer in agreement to measured data for the same endpoint compared to predictions using measured log K_{ow} values as inputs.

A2.3.1 Monostyrenated phenol

SMILES: **c1(O)c(C(C)c2ccccc2)cccc1** (styrenated subgroup in the *ortho* position)[31]
CHEM:
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: $C_{14}H_{14}O$
MOL WT: 198.27
Log K_{ow}: 3.67 (KowWin estimate)
Melting Pt:
Water Sol: 231 mg/l (measured value; Lange, 2005a)

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/l (ppm)
Neutral Organic SAR: (Baseline Toxicity)	Fish	14-day	LC_{50}	9.347
Phenols:	Fish	96-hour	LC_{50}	2.726
Phenols:	Daphnid	48-hour	LC_{50}	2.214
Phenols:	Green Algae	96-hour	EC_{50}	3.276
Phenols:	Fish	30-day	ChV	0.400
Phenols:	Fish	90-day	ChV	0.042
Phenols:	Daphnid	21-day	ChV	0.296
Phenols:	Green Algae	96-hour	ChV	0.860

Fish and *Daphnid* acute toxicity log K_{ow} cutoff: 7.0
Green algal EC_{50} toxicity log K_{ow} cutoff: 7.0
Chronic toxicity log K_{ow} cutoff: 9.0
MW cutoff: 1,000

A2.3.2a 2,4- Distyrenated phenol

SMILES: **c1(O)c(C(C)c2ccccc2)cc(C(C)c3ccccc3)cc1**

---

[31] The same results are reported by ECOSAR for c1(O)ccc(C(C)c2ccccc2)cc1 (the monostyrenated phenol with the styrenated subgroup in the *para* position).

CHEM:
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: $C_{22}H_{22}O$
MOL WT: 302.42
Log K_{ow}: 5.83 (KowWin estimate)
Melting Pt:
Water Sol: 0.665 mg/l (measured value; Lange, 2005b)

ECOSAR Class	**Organism**	**Duration**	**End Pt**	**Predicted mg/l (ppm)**
Neutral Organic SAR: (Baseline Toxicity)	Fish	14-day	LC_{50}	0.187
Phenols:	Fish	96-hour	LC_{50}	0.194
Phenols:	Daphnid	48-hour	LC_{50}	0.442
Phenols:	Green Algae	96-hour	EC_{50}	0.061
Phenols:	Fish	30-day	ChV	0.027
Phenols:	Fish	90-day	ChV	0.007
Phenols:	Daphnid	21-day	ChV	0.021
Phenols:	Green Algae	96-hour	ChV	0.056

Fish and *Daphnid* acute toxicity log K_{ow} cutoff: 7.0
Green algal EC_{50} toxicity log K_{ow} cutoff: 7.0
Chronic toxicity log K_{ow} cutoff: 9.0
MW cutoff: 1,000

A2.3.2b 2,6-Distyrenated phenol

SMILES: c1(C(C)c3ccccc3)c(O)c(C(C)c2ccccc2)ccc1
CHEM:
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: $C_{22}H_{22}O$
MOL WT: 302.42
Log K_{ow}: 4.98 (KowWin estimate)
Melting Pt:
Water Sol: 0.665 mg/l (calculated value; Lange, 2005b)

ECOSAR Class	**Organism**	**Duration**	**End Pt**	**Predicted mg/l (ppm)**
Neutral Organic SAR: (Baseline Toxicity)	Fish	14-day	LC_{50}	1.030*
Phenols:	Fish	96-hour	LC_{50}	0.649
Phenols:	Daphnid	48-hour	LC_{50}	0.984*
Phenols:	Green Algae	96-hour	EC_{50}	0.346
Phenols:	Fish	30-day	ChV	0.093
Phenols:	Fish	90-day	ChV	0.017
Phenols:	Daphnid	21-day	ChV	0.071
Phenols:	Green Algae	96-hour	ChV	0.194

*Chemical may not be soluble enough to measure this predicted effect.

Fish and *Daphnid* acute toxicity log K_{ow} cutoff: 7.0
Green algal EC_{50} toxicity log K_{ow} cutoff: 7.0
Chronic toxicity log K_{ow} cutoff: 9.0
MW cutoff: 1,000

A2.3.3 Tristyrenated phenol

SMILES: **c(ccc1C(-c(cc(c2O)C(-c(ccc3)cc3)C)cc2C(-c(ccc4)cc4)C)C)cc1**
CHEM:
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: $C_{30}H_{30}O$
MOL WT: 406.57
Log K_{ow}: 7.13 (KowWin estimate)
Melting Pt:
Water Sol: 0.01058 mg/l (ECOSAR calculated)

ECOSAR Class	**Organism**	**Duration**	**End Pt**	**Predicted mg/l (ppm)**
Neutral Organic SAR: (Baseline Toxicity)	Fish	14-day	LC_{50}	0.019*
Phenols:	Fish	96-hour	LC_{50}	0.041*
Phenols:	Daphnid	48-hour	LC_{50}	0.175*
Phenols:	Green Algae	96-hour	EC_{50}	0.006
Phenols:	Fish	30-day	ChV	0.006
Phenols:	Fish	90-day	ChV	0.002
Phenols:	Daphnid	21-day	ChV	0.005
Phenols:	Green Algae	96-hour	ChV	0.011*

*Chemical may not be soluble enough to measure this predicted effect.

Fish and *Daphnid* acute toxicity log K_{ow} cutoff: 7.0
Green algal EC_{50} toxicity log K_{ow} cutoff: 7.0
Chronic toxicity log K_{ow} cutoff: 9.0
MW cutoff: 1,000

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