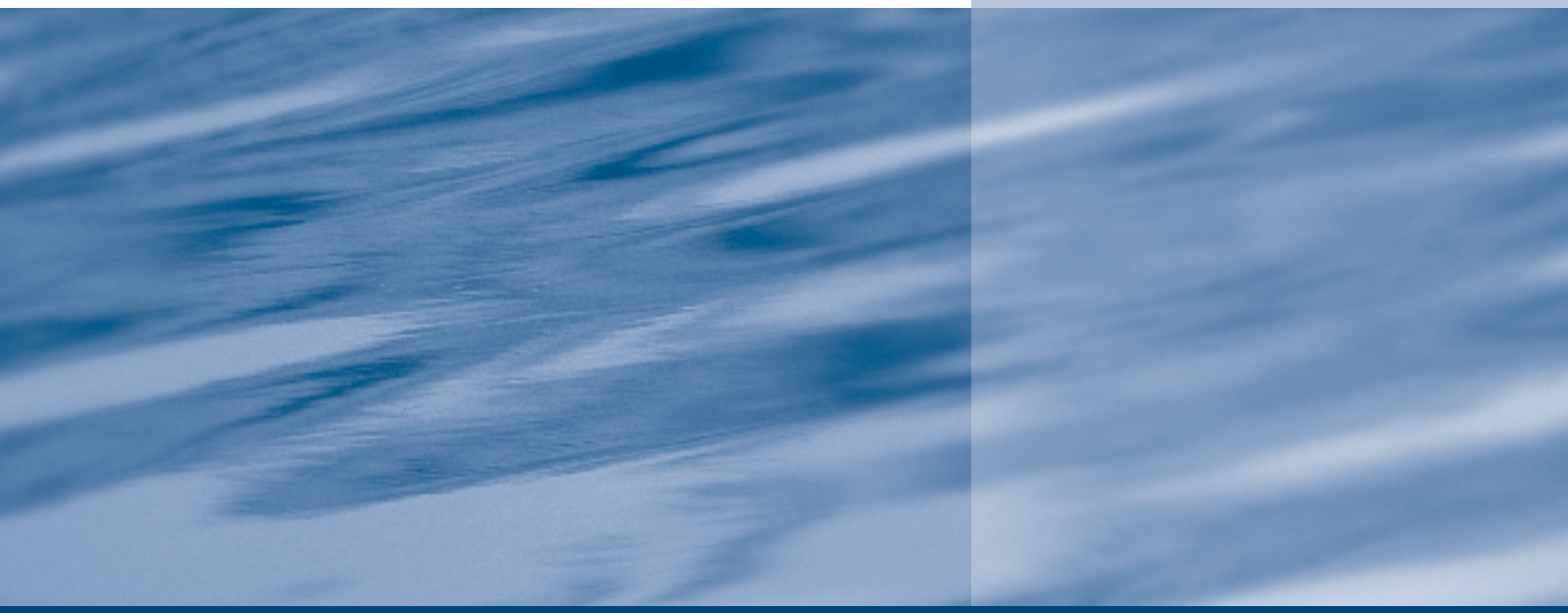

www.environment-agency.gov.uk

Prioritisation of Alkylphenols for Environmental Risk Assessment

ENVIRONMENT AGENCY

The Environment Agency is the leading public body protecting and improving the environment in England and Wales.

It's our job to make sure that air, land and water are looked after by everyone in today's society, so that tomorrow's generations inherit a cleaner, healthier world.

Our work includes tackling flooding and pollution incidents, reducing industry's impacts on the environment, cleaning up rivers, coastal waters and contaminated land, and improving wildlife habitats.

This report is the result of research commissioned and funded by the Environment Agency's Science Programme.

Published by:
Environment Agency, Rio House, Waterside Drive, Aztec West, Almondsbury, Bristol, BS32 4UD
Tel: 01454 624400 Fax: 01454 624409
www.environment-agency.gov.uk

ISBN: 1 84432 369 2

This report is printed on Cyclus Print, a 100% recycled stock, which is 100% post consumer waste and is totally chlorine free. Water used is treated and in most cases returned to source in better condition than removed.

Further copies of this report are available from:
The Environment Agency's National Customer Contact Centre by emailing enquiries@environment-agency.gov.uk or by telephoning 08708 506506.

Author(s):
D Brooke, M Crookes, I Johnson, R Mitchell & C Watts

Dissemination Status:
Publicly available

Keywords:
Nonylphenol, octylphenol, alkylphenol, endocrine disruption, PBT, hazard, risk, prioritisation

Research Contractor:
Building Research Establishment, Garston, Watford WD25 9XX
Tel: +44 (0)1923 664862

WRc-NSF Ltd, Medmenham, Marlow, Buckinghamshire SL7 2HD
Tel: +44 (0)1491 636 500

Environment Agency's Project Manager:
S Dungey
Chemicals Assessment Unit, Wallingford OX10 8BD
Tel: +44(0)1491 828 557

Product Code:
SCHO0205BINF-E-P

Science at the Environment Agency

Science underpins the work of the Environment Agency, by providing an up to date understanding of the world about us, and helping us to develop monitoring tools and techniques to manage our environment as efficiently as possible.

The work of the Science Group is a key ingredient in the partnership between research, policy and operations that enables the Agency to protect and restore our environment.

The Environment Agency's Science Group focuses on five main areas of activity:

- **Setting the agenda**: To identify the strategic science needs of the Agency to inform its advisory and regulatory roles.
- **Sponsoring science**: To fund people and projects in response to the needs identified by the agenda setting.
- **Managing science**: To ensure that each project we fund is fit for purpose and that it is executed according to international scientific standards.
- **Carrying out science**: To undertake the research itself, by those best placed to do it – either by in-house Agency scientists, or by contracting it out to universities, research institutes or consultancies.
- **Providing advice**: To ensure that the knowledge, tools and techniques generated by the science programme are taken up by relevant decision makers, policy makers and operational staff.

Professor Mike Depledge Head of Science

Executive summary

Background

The United Kingdom nominated nonylphenol and 4-nonylphenol (branched) for inclusion on the second priority list of Council Regulation (EEC) 793/93 (the Existing Substances Regulation or ESR) in 1995. The comprehensive risk assessment that followed identified a large number of risks to the environment.

Other alkylphenols (particularly octylphenol) were identified as the only alternatives to nonylphenol where it is used as an intermediate for other derivatives (e.g. phenol/formaldehyde resins, phenolic oximes and plastic stabilisers). The risk reduction strategy considered that it was inappropriate to recommend discontinuation of these uses until further information on the comparative level of risks was available for the possible replacements.

This report was commissioned to review and prioritise for further assessment other alkylphenols that might be potential replacements for nonylphenol, in support of the nonylphenol risk reduction strategy.

Main objectives

An initial list of alkylphenols was compiled by searching relevant chemical databases and consulting the Conseil Européen des Phénols Alkylés et Derivés (CEPAD). Industry identified potential substitutes for nonylphenol from this list, and datasheets were prepared for the selected substances covering parameters such as production tonnages, use pattern, physicochemical properties, persistence (P), bioaccumulation (B) and toxicity (T). The substances were then prioritised in terms of their current availability and suitability as replacements, and their hazard – especially PBT – profile.

Results

A number of significant factors are apparent:

- On the basis of data provided by industry only a limited number of candidate alkylphenols are commercially important at the moment, and very few are produced or used at quantities greater than 1,000 tonnes/year in Europe.
- Only a few have appropriate physicochemical properties for consideration as potential substitutes for nonylphenol; even then changes may be needed in production and processing methods compared with nonylphenol.

- There are significant variations in the cost of these substances owing to availability of feedstock.
- There is very little information about environmental occurrence.
- In general terms the amount of hazard data (e.g. for biodegradation, bioaccumulation and toxicity) is limited, although it is apparent that longer chain length 4-alkylphenols are generally more toxic to aquatic organisms than those with short chain lengths.

Conclusions

A short-list of possible replacement substances has been compiled and the following recommendations are made:

1. A full environmental risk assessment should be performed for 4-*tert*-octylphenol (CAS no. 140-66-9) and dodecylphenol (branched) (CAS nos. 121158-58-5 & 74499-35-7) as a priority.

2. Risk assessments should also be undertaken for the remaining candidate nonylphenol substitutes, with priority given to:

   - 4-*tert*-pentylphenol (CAS no. 80-46-6)
   - 2,4-di-*tert*-butylphenol (CAS no. 96-76-4)
   - 2,6-di-*tert*-butylphenol (CAS no. 128-39-2).

3. Other commercially important substances with a PBT profile of potential concern could be considered for risk assessment too, although since their supply tonnage appears to be low, these are of lower priority compared with the substances above:

   - 2,4-di-*tert*-pentylphenol (CAS no. 120-95-6)
   - 2,4-dinonylphenol (branched) (CAS no. 84852-14-2)
   - styrenated phenol (CAS no. 61788-44-1).

4. 4-*tert*-Heptylphenol (CAS no. 1987-50-4) should also be considered in any assessment of 4-*tert*-pentylphenol. Consideration could also be given to obtaining more information on 4-cumylphenol (CAS no. 599-64-4).

5. The available data are insufficient to allow even a basic assessment for most of these substances at present, and this needs to be addressed first. One way might be to encourage sponsorship through international hazard assessment initiatives, or data call-in under the ESR.

Contents **Page**

Executive summary **iv**

1 Introduction **1**

1.1 Background 1

1.2 Data sources 2

2 Substances considered in this review **4**

2.1 Identification of alkylphenols 4

2.2 Substitution of nonylphenol by other alkylphenols 7

3 Data gathering for candidate substances **9**

3.1 Supply volume 9

3.2 Use data 12

3.3 Physicochemical properties 13

3.4 Economic and other factors 14

3.5 Environmental concentrations 15

3.6 Persistence 17

3.7 Bioaccumulation 18

3.8 Ecotoxicity data 19

3.9 PBT assessment 26

3.10 Summary of fate and effect data 26

4 Analysis and discussion **40**

4.1 General overview of the data 40

4.2 Hazard profiles for possible substitute alkylphenols 40

5 Conclusions **43**

6 Recommendations **45**

References **47**

Annex I Alkylphenol datasheets **50**

Glossary of terms **69**

List of abbreviations **70**

Annex II to this report contains **confidential industry data** relating to European supply tonnage and use pattern. This annex is a separate document, and can be made available to regulatory authorities on request to the Project Manager.

List of tables

Table 1.1 Summary of the primary data sources used to obtain information on alkylphenols 3

Table 2.1 List of alkylphenols (APs) potentially on the market 4

Table 2.2 Alkylphenols that can be used to substitute nonylphenol 8

Table 3.1 Summary of data on the commercial relevance of alkylphenols 10

Table 3.2 Production and use data for alkylphenols of commercial interest 11

Table 3.3 Volumes of substances (excluding ethoxylates) produced from alkylphenols 12

Table 3.4 Summary of the problems of using alkylphenols as substitutes for nonylphenol to produce ethoxylate surfactants 13

Table 3.5 Summary of the problems of using alkylphenols as substitutes for nonylphenol for production of resins, plastics, stabilisers, etc. 14

Table 3.6 Summary of surface water monitoring data for alkylphenols (as dissolved concentrations) 16

Table 3.7 Summary of data on alkylphenol (and ethoxylate) concentrations in River Elbe catchment sediments 17

Table 3.8 Comparison of the lowest reliable acute and chronic toxicity data for four data rich alkylphenols 21

Table 3.9 Summary of 96-hr NOECs of alkylphenols for mortality of juvenile *Daphnia magna* 24

Table 3.10 Summary of concentrations of alkylphenols causing mortality of *Crangon septemspinosa* 24

Table 3.11 Summary fate and hazard data on identified alkylphenols 27

Table 4.1 Hazard profiles for nonylphenol and potential substitute alkylphenols 41

1 Introduction

1.1 Background

The United Kingdom nominated nonylphenol and 4-nonylphenol (branched) for inclusion on the second priority list of Council Regulation (EEC) 793/93[1] (the Existing Substances Regulation or ESR) in 1995. This was based on general concerns about aquatic toxicity and biodegradation, and during the assessment process specific concerns were also raised about the effects that nonylphenol can have on the endocrine system. The comprehensive risk assessment that followed identified a large number of risks to the environment (as well as some specific risks to workers using speciality paints) (ECB, 1999). The uses of concern included both the production of nonylphenol itself and its formulation and use in the manufacture of other products. In particular, nonylphenol is used to make ethoxylate derivatives, and the degradation of these substances represents the main source of nonylphenol in the environment. Risks were predicted for both the aquatic and terrestrial compartments, and to predators through accumulation in the food chain.

The accompanying risk reduction strategy proposed a number of policy measures to reduce emissions from those uses giving rise to the principal sources of environmental exposure (DETR, 1999). In summary, these are:

1. Comprehensive phase-outs under Directive 76/769/EEC of those uses that contribute most to the regional concentration and/or for which less harmful alternatives to nonylphenol and nonylphenol ethoxylates are known to be available. These include, for example, use of ethoxylates in cleaning products and cosmetics. The ban will come into force early in 2005. It was recognised that derogations could be accepted for some specific applications.

2. An environmental quality standard (EQS) for the remaining uses. For all facilities that will be licensed under the Industrial Pollution Prevention and Control (IPPC) Directive 96/61/EEC, the EQS was expected to be included in the IPPC operating licence. For non-IPPC facilities, the EQS will have to be established through other regulatory means (e.g. the Water Framework Directive 2000/60/EC). It was proposed that risks associated with uses not covered by IPPC could be reduced sufficiently in the short term by voluntary agreements.

A key aspect considered in the risk reduction strategy was the replacement of nonylphenols with other compounds. Long chain (fatty) alcohol ethoxylates were identified as the main substitutes for nonylphenol ethoxylates. These are generally considered to be less environmentally harmful, and a hazard assessment is currently under way in the Organisation for Economic Co-operation and Development (OECD) Screening Initial Data Set (SIDS)

[1] Official Journal No L 084, 05/04/1993 p. 0001–0075

programme (led by industry with the UK acting as the sponsor country) (http://cs3-hq.oecd.org/scripts/hpv/).

However, other alkylphenols (particularly octylphenol) were suggested to be the only alternative to nonylphenol where it is used as an intermediate for derivatives other than ethoxylates (e.g. phenol/formaldehyde resins, phenolic oximes and plastic stabilisers). The risk reduction report concluded that discontinuation of the use of nonylphenol as a chemical intermediate in these applications could not be recommended until further information on the comparative levels of risks of the alternatives is available.

The alkylphenol group has already attracted considerable attention by other regulatory fora. For example, some have been identified by OSPAR[2] contracting parties as substances for priority action (OSPAR, 2000). These substances were prioritised based on an evaluation of the data on their persistence (P), bioaccumulation potential (B) and toxicity (T) against defined thresholds for these criteria. The substances are:

- 4-*tert*-octylphenol (CAS no. 140-66-9)
- 2,4,6-tris(1,1-dimethylethyl)phenol (CAS no. 732-26-3).

In addition, both nonylphenol and 4-*tert*-octylphenol have been prioritised for voluntary emission reduction action by the UK Government's Chemicals Stakeholder Forum (further details can be obtained from http://www.defra.gov.uk/environment/chemicals/csf/index.htm).

There is therefore an urgent need to identify additional alkylphenols that could be potential replacements for nonylphenol so that their environmental impact can be properly assessed. This is the purpose of this report. Candidate substances have been identified and are prioritised in terms of their current availability and suitability as replacements, and their hazard profile. The information is intended for use by the Environment Agency's Chemicals Policy function and the Department for Environment, Food & Rural Affairs to inform future assessment and monitoring priorities and wider policy on alkylphenols.

1.2 Data sources

An initial list of alkylphenols was compiled by searching relevant chemical databases. Further substances were identified following discussions with the Conseil Européen des Phénols Alkylés et Derivés (CEPAD).[3] The primary data sources used to collect information on alkylphenols are summarised in Table 1.1.

[2] The OSPAR Commission was set up to protect the marine environment of the north-east Atlantic.

[3] CEPAD is the European Council for Alkylphenols and Derivatives. It is a trade association representing the major (although not necessarily all) producers of alkylphenols, and is part of the European chemical industry body CEFIC. It also represents some of the users.

The Environment Agency would like to thank CEPAD for its very helpful co-operation in the production of this report.

An initial evaluation of these sources indicated that the quantity of data for the different substances varied considerably; most data were available for those listed in IUCLID.[4] Information on many of the alkylphenols identified by CEPAD (which were not in IUCLID) was generally absent or very limited.

Table 1.1 Summary of the primary data sources used to obtain information on alkylphenols

Subject area	Data sources used
Quantities used	Confidential IUCLID (2000); CEPAD
Uses (industrial and functional)	Confidential IUCLID (2000); CEPAD; OECD SIDS reports
Physicochemical data	Non-confidential IUCLID CD (2000); SASOL (2001) Safety Data Sheets; Robust Summaries submitted to USEPA (2001); Environment Agency environmental quality standard (EQS) reports;[a] BUA (2001); OECD SIDS reports
Environmental fate and behaviour	Non-confidential IUCLID CD (2000); Environment Agency EQS reports[a]; BUA (2001); OECD SIDS reports
Environmental concentration data	European Environment Agency data; Environment Agency EQS reports;[a] Data supplied by CEPAD; OECD SIDS reports
Aquatic toxicity data	Non-confidential IUCLID CD (2000); US EPA Acquire database; OECD SIDS reports; Environment Agency EQS reports;[a] KEMI (2000)[b]
Terrestrial toxicity data	Non-confidential IUCLID CD (2000); OECD SIDS reports

Notes: [a] Methylphenols (cresols) and octylphenol
[b] Butylphenols and octylphenols

If data were not available from the primary data sources only limited additional searching was carried out. Other sources of information included the in-house NCET database at WRc-NSF Ltd, Current Contents CD-ROM and relevant Internet sites operated by the Environment Agency, RIVM in the Netherlands, Environment Canada, the United States Environmental Protection Agency and the OECD. All of these proved valuable, particularly since the amount of information available for most alkylphenols is limited. **Note**: This search was conducted during 2002; additional data might have become available since this time, but they have not been taken into account for this report.

[4] **I**nternational **U**niform **C**hemica**L** **I**nformation **D**atabase – containing unvalidated tonnage, use pattern, property and hazard information for 2,604 EU high production volume (HPV) chemicals, submitted by industry under the ESR. A HPV substance is one that was produced or imported by at least one company at 1,000 tonnes per year or above at least once in 1990–1994.

2 Substances considered in this review

2.1 Identification of alkylphenols

A wide variety of alkylphenol structures are possible, but many are not commercially important or relevant to this review. A list of alkylphenols that appear to have been produced commercially at some time is provided in Table 2.1. This list was compiled after searching the data sources outlined in Section 1.2, with further substances added following discussions with CEPAD. Mono-substituted alkylphenols have typical alkyl chains ranging in length from 1 to 12 carbon atoms. Note that a different naming system for the substitution position (*ortho*-, *meta*- and *para*-) can also be used (these are not all listed separately as synonyms).

Table 2.1 List of alkylphenols (APs) potentially on the market

Substance	CAS No.	Formula	Common synonyms (not exhaustive)
C_1 APs			
Methylphenols	1319-77-3	C_7H_8O	Cresols
2-Methylphenol	95-48-7	C_7H_8O	o-cresol
3-Methylphenol	108-39-4	C_7H_8O	m-cresol
4-Methylphenol	106-44-5	C_7H_8O	p-cresol
C_2 APs			
2-Ethylphenol	90-00-6	$C_8H_{10}O$	1-ethyl-2-hydroxybenzene
4-Ethylphenol	123-07-09	$C_8H_{10}O$	1-ethyl-4-hydroxybenzene
Dimethylphenols	1300-71-6	$C_8H_{10}O$	Xylenols
2,6-Dimethylphenol	576-26-1	$C_8H_{10}O$	2,6-xylenol
3,5-Dimethylphenol	108-68-9	$C_8H_{10}O$	3,5-xylenol
C_3 APs			
2-Isopropylphenol	88-69-7	$C_9H_{12}O$	-
2,3,6-Trimethylphenol	2416-94-6	$C_9H_{12}O$	-
C_4 APs			
2-*tert*-Butylphenol	88-18-6	$C_{10}H_{14}O$	-
3-*tert*-Butylphenol	585-34-2	$C_{10}H_{14}O$	-
4-*tert*-Butylphenol	98-54-4	$C_{10}H_{14}O$	4-(2-methyl-2-propyl)phenol
2-*sec*-Butylphenol	89-72-5	$C_{10}H_{14}O$	-
4-*sec*-Butylphenol	99-71-8	$C_{10}H_{14}O$	4-(2-butyl)phenol

Table continued overleaf

Table 2.1 continued

Substance	CAS No.	Formula	Common synonyms (not exhaustive)
C_5 APs			
2-*tert*-Pentylphenol	3279-27-4	$C_{11}H_{16}O$	o-*tert*-amylphenol
4-*tert*-Pentylphenol	80-46-6	$C_{11}H_{16}O$	p-(1,1-dimethylpropyl)-phenol, p-*tert*-amylphenol, 4-(2-methyl-2-butyl)phenol
2-*tert*-Butyl-p-methylphenol	2409-55-4	$C_{11}H_{16}O$	2-(1,1-dimethylethyl)-4-methyl-phenol
C_6 APs			
4-Hexylphenol	2446-69-7	$C_{12}H_{18}O$	-
2-Cyclohexylphenol	119-42-6	$C_{12}H_{18}O$	-
2-*tert*-Butyl-4-ethyl-phenol	96-70-8	$C_{12}H_{18}O$	-
C_7 APs			
4-Heptylphenol	1987-50-4	$C_{13}H_{20}O$	-
C_8 APs			
Octylphenols	27193-28-8	$C_{14}H_{22}O$	-
4-*tert*-Octylphenol	140-66-9	$C_{14}H_{22}O$	4-(1,1,3,3-tetramethylbutyl)phenol
4-Octylphenol	1806-26-4	$C_{14}H_{22}O$	-
Isooctylphenol	11081-15-5	$C_{14}H_{22}O$	-
2,4-Di-*tert*-butylphenol	96-76-4	$C_{14}H_{22}O$	-
2,6-Di-*tert*-butylphenol	128-39-2	$C_{14}H_{22}O$	-
C_{10} APs			
2,4-Di-*tert*-pentyl-phenol	120-95-6	$C_{16}H_{26}O$	2,4-bis(1,1-dimethylpropyl)-phenol, 2,4-di-*tert*-amylphenol
2,6-Di-*tert*-butyl-4-ethyl phenol	4130-42-1	$C_{16}H_{26}O$	-
C_{12} APs			
Dodecylphenol, mixed isomers	27193-86-8	$C_{18}H_{30}O$	Tetrapropenylphenol
4-Dodecylphenol	104-43-8	$C_{18}H_{30}O$	-
Phenol, dodecyl-branched	121158-58-5	$C_{18}H_{30}O$	-
Phenol, (tetrapropenyl) derivatives	74499-35-7	$C_{18}H_{30}O$	
Isododecylphenol	11067-80-4	$C_{18}H_{30}O$	-

Table continued overleaf

Table 2.1 continued

Substance	CAS No.	Formula	Common synonyms (not exhaustive)
C_{12} APs (continued)			
2,4,6-Tri-*tert*-butylphenol	732-26-3	$C_{18}H_{30}O$	2,4,6-tris(1,1-dimethylethyl)phenol
2,4,6-Tri-*sec*-butylphenol	5892-47-7	$C_{18}H_{30}O$	-
4-*sec*-Butyl-2,6-di-*tert*-butylphenol	17540-75-9	$C_{18}H_{30}O$	2,6-di-*tert*-butyl-4-*sec*-butylphenol
Other APs			
2,4-Dinonylphenol	137-99-5	$C_{24}H_{42}O$	-
Dinonylphenol	1323-65-5	$C_{24}H_{42}O$	-
Phenol, 2,4-dinonyl branched	84852-14-2	$C_{24}H_{42}O$	-
2,6-Di-*tert*-butyl-p-cresol	128-37-0	$C_{24}H_{42}O$	Butylated hydroxytoluene (BHT)
4-Hexyldecylphenol	2589-78-8	$C_{22}H_{38}O$	
2,6-Di-*tert*-butyl-4-nonyl phenol	4306-88-1	$C_{23}H_{40}O$	-
Bis(*tert*-butyl)dodecyl-phenol	68025-37-6	$C_{26}H_{46}O$	-
Phenol, isopropylated	90480-88-9		-
Phenol, isobutylated	68610-06-0		-
Phenol, C_{18-30} alkyl derivatives[5]	68784-24-7	Unclear	-
Aryl phenols (not covered in detail by this review)			
2,4,6-Tris(1-phenylethyl) phenol	18254-13-2	$C_{30}H_{30}O$	-
Phenol, styrenated	61788-44-1	Complex	-
Cumylphenol	27576-86-9	$C_{15}H_{16}O$	1-methyl-1-phenylethyl phenol
4-Cumylphenol	599-64-4	$C_{15}H_{16}O$	4-alpha-cumylphenol
2-Cumylphenol	18168-40-6	$C_{15}H_{16}O$	1-alpha-cumylphenol
2,4-Di-cumenephenol	Unclear	$C_{20}H_{26}O$	-

A superficial data search was undertaken for all of these substances using the data sources listed in the previous section; most of the information came from secondary sources such as IUCLID (2000). The results of this are shown in Table 3.11.

[5] High molecular weight alkylphenols are used in certain applications (e.g. C14-18 or higher alpha-olefin derived alkylphenols are used to make salicylate lubricant additives), but these do not have any real potential to replace nonylphenol and so are not considered in any detail in this report.

2.2 Substitution of nonylphenol by other alkylphenols

Consideration was given to the possibility of using other alkylphenols as a substitute for nonylphenol in all of its major uses. CEPAD provided the information for this section (personal communication, 2002), and the information has not been verified with other sources.

Although other alkylphenols were not identified as a *likely* substitute for nonylphenol in ethoxylate production during the risk management work, the similar chemical nature of some does not rule out the possibility. Nonylphenol (NP) can in fact be substituted by 4-*tert*-octylphenol (OP) in most ethoxylate uses. Although OP is widely used in the USA for the production of ethoxylates, its use for the production of ethoxylates in Europe is limited to specialist applications at present. The main reasons are:

- the higher price due to the limited availability of octene feedstock in Europe;

- handling difficulties: whereas NP is a liquid, OP is a solid at room temperature and therefore pumping is only possible at temperatures around 90°C.

In addition, many uses of nonylphenol ethoxylates can be substituted by the use of long chain (fatty) alcohol ethoxylates. These are significantly cheaper than octylphenol ethoxylates.

These alcohols are not a substitute for use in phenol/formaldehyde resins due to the difference in chemical structures and properties. In general, where NP is used as an intermediate for other (non-ethoxylate) products, only alkylphenols that have similar physical and chemical properties to NP can be used as substitutes (if at all). The three major types of use for NP are shown in Table 2.2, together with an indication of which alkylphenols could be used as a substitute for NP based on acceptable properties of the products for these uses.

Table 2.2 Alkylphenols that can be used to substitute nonylphenol

Uses	Potential alternatives
1 Nonylphenol ethoxylates	
• Cleaning/washing agents	4-*tert*-octylphenol
• Construction materials and additives	4-*tert*-octylphenol
• Cosmetics	4-*tert*-octylphenol
• Dust binding agents	4-*tert*-octylphenol
• Flotation agents	4-*tert*-octylphenol
• Foaming agents	4-*tert*-octylphenol
• Intermediates	4-*tert*-octylphenol
• Pesticides/veterinary medicines	4-*tert*-octylphenol, dodecylphenol
• Surface active agents	4-*tert*-octylphenol, dodecylphenol
• Others	4-*tert*-octylphenol
Uses	**Potential alternatives**
2 Resins, plastics, stabilisers, etc.	
• Production of phenol/ formaldehyde resins Note: possible substitution strongly depends on the final use and required properties of the resins.	4-*tert*-butylphenol, 4-*tert*-octylphenol, 4-*tert*-pentylphenol [4-cumylphenol (*not* an alkylphenol)]
• Intermediate in the production of tris-(4-nonylphenyl)phosphite (TNPP)	None
• Catalyst in the curing of epoxy resins	None in general, perhaps dodecylphenol
• Intermediate in the production of other plastic stabilisers	2-*tert*-butylphenol, 2,4-di-*tert*-butylphenol, 2,6-di-*tert*-butylphenol
3 Phenolic oximes	The only known European production site is in Ireland. The oximes are mainly exported outside Europe for use in copper mining. To the best of CEPAD's knowledge, 4-*tert*-octylphenol cannot be used for the production of phenolic oximes. Dodecylphenol has been investigated for the same use, but the costs are much higher.

3 Data gathering for candidate substances

From Table 2.2, the potential substitutes in one or more applications are 2-*tert*-butylphenol, 4-*tert*-butylphenol, 4-*tert*-pentylphenol, 4-*tert*-octylphenol, dodecylphenol, 4-cumylphenol (though this is not an alkylphenol), 2,4-di-*tert*-butylphenol and 2,6-di-*tert*-butylphenol. Information was sought from industry as to which substances on the initial list (Table 2.1) were currently being produced on a commercial basis. The results of this are shown in Table 3.1. Where there were sufficient data or where particular comment had been made by industry to merit inclusion of a substance, datasheets were compiled for these particular (16) substances to assist in later considerations. These are provided in Annex I and II to this report (Annex II contains confidential data on supply volume and use pattern, and is not included in this document). Note that 4-*tert*-butylphenol is a fourth priority list substance under the ESR, and so it is currently undergoing an in-depth risk assessment for environmental as well as human health endpoints. It is therefore not necessary to prioritise this substance for further assessment.

3.1 Supply volume

Data on the quantities currently used (production plus imports minus exports) in Western Europe (i.e. EU countries along with Norway and Switzerland) and the industrial and functional uses of the alkylphenols identified in Table 2.1 were initially obtained from the confidential IUCLID. However, in many cases this information (summarised in Annex II) related to 1990–1994, and more recent data were obtained where possible from industry through CEPAD. Only two companies are now producing a range of alkylphenols, which represents a major change from the situation in the mid-1990s.

Table 3.1 summarises CEPAD data (personal communication, 2002) on the relative commercial importance of 30 different alkylphenols (including one arylphenol). Sixteen substances are currently believed to be commercially relevant by CEPAD, and 10 of these are produced at volumes exceeding 1,000 tonnes/year (i.e. generally recognised as ‘high production volume’ or HPV substances). These are highlighted in the table in bold. Once again, this information has not been verified with other sources.[6]

All possible replacements for nonylphenol are currently considered to come from the ‘commercially important’ sub-group of alkylphenols. With the exception of 4-*tert*-pentylphenol, these are all produced at high tonnage (data

[6] It became apparent towards the end of this project that the lubricant industry might be major users of some of the substances. For example, 4-*tert*-heptylphenol was considered to be commercially unimportant by CEPAD, yet the industry in the USA has submitted a test plan under the US HPV Chemical Challenge programme (which implies a major use in North America, which could be reflected in the EU, at least in imported products). The tonnage information might therefore not reflect the entire EU tonnage.

were not provided for 4-cumylphenol). This excludes substances such as styrenated phenol.

Table 3.1 Summary of data on the commercial relevance of alkylphenols

Substance	CAS No.	Commercially important?		HPV?
		Yes	No	
2-Isopropylphenol	88-69-7		√	No
2-*tert*-Butylphenol	**88-18-6**	√		**Yes**
4-*tert*-Butylphenol	**98-54-4**	√		**Yes**
2-*sec*-Butylphenol	89-72-5	√		No
4-*tert*-Pentylphenol	80-46-6	√		No
2-*tert*-Butyl-p-methylphenol	**2409-55-4**	√		**Yes**
Isooctylphenol	11081-15-5		√	No
4-*tert*-Octylphenol	**140-66-9**	√		**Yes**
2,4-Di-*tert*-butylphenol	**96-76-4**	√		**Yes**
2,6-Di-*tert*-butylphenol	**128-39-2**	√		**Yes**
2,6-Di-*tert*-butyl-p-cresol (BHT)	**128-37-0**	√		**Yes**
2,4-Di-*tert*-pentylphenol	120-95-6	√		No
2,6-Di-*tert*-butyl-4-ethyl phenol	4130-42-1		√	No
2,4,6-Tri-*tert*-butylphenol	732-26-3		√	No
2,4,6-Tri-*sec*-butylphenol	5892-47-7		√	No
4-*sec*-Butyl-2,6-di-*tert*-butylphenol	17540-75-9		√	No
4-Dodecylphenol	104-43-8		√	No
Isododecylphenol	11067-80-4		√	No
Dodecyl (branched)*	**121158-58-5 74499-35-7**	√		**Yes**
2,4-Dinonylphenol	137-99-5	√		No
Dinonylphenol	1323-65-5	√		No
p-Hexyldecylphenol	2589-78-8		√	No
2,6-Di-*tert*-butyl-4-nonyl phenol	4306-88-1		√	No
2,4,6-Tris(1-phenylethyl) phenol	18254-13-2		√	No
Bis(*tert*-butyl)dodecylphenol	68025-37-6		√	No
Phenol, isobutylenated	68610-06-0		√	No
Phenol, C_{18-30} alkyl derivatives	68784-24-7		√	No
Phenol, 2,4-dinonyl branched	**84852-14-2**	√		**Yes**
Phenol, isopropylated	**90480-88-9**	√		**Yes**
Phenol, styrenated	61788-44-1	√		No

* This term is used in this document to describe the commercial substance: there appear to be at least two CAS numbers in commercial use.

Table 3.2 summarises data on the 1999 production quantity of some of the commercially important alkylphenols (and one arylphenol) (CEPAD, personal communication, 2002).

Table 3.2 Production and use data for alkylphenols of commercial interest

Substance	Volumes in Western Europe (tonnes/year)			
	Produced	**Exported**	**Imported**	**Total**
Nonylphenol (1997 data)	73,500	3,500	8,500	78,500
Other Alkylphenols (1999 data)				
2-*tert*-Butylphenol	1,200	?	?	?
4-*tert*-Butylphenol	20,000	1,000	1,000	20,000
2-sec-Butylphenol	500	?	?	?
4-*tert*-Pentylphenol	300	100	200	400
4-*tert*-Octylphenol*	22,633	1,500	375	21,508
2,4-Di-*tert*-butylphenol	13,000	-	-	13,000
2,6-Di-*tert*-butylphenol	15,000	-	-	15,000
2,4,6-Tri-*tert*-butyl-phenol	10	?	?	?
Phenol, styrenated	<100	-	-	<100#
2-Isopropylphenol	100	?	?	?
Dodecylphenol, branched*	Confidential	Confidential	Confidential	10,000–50,000

* Data for 2001

The Environment Agency is aware that there are a number of manufacturers of styrenated phenol. It is not clear how many of these are represented by CEPAD, so the tonnage could be higher than this figure.

Data were not presented for the following HPV substances (with CAS numbers):

- 2-*tert*-butyl-p-methylphenol 2409-55-4
- 2,6-di-*tert*-butyl-p-cresol (BHT) 128-37-0[7]
- isopropylated phenol 90480-88-9
- 2,4-dinonylphenol (branched) 84852 -14-2
  (presumably related to 2,4-dinonylphenol and dinonylphenol)

or for one other alkylphenol that is considered commercially important:

- 2,4-di-*tert*-pentylphenol 120-95-6.

Note that the substance identified by OSPAR as a priority hazardous substance (2,4,6-tri-*tert*-butylphenol) is not considered commercially important.

[7] A hazard assessment for BHT has recently been agreed by the OECD, but the results are not considered here.

3.2 Use data

Table 3.3 presents tonnage information for the products currently produced from the alkylphenols. Note that data have not been presented for all the substances listed in Table 3.1 (CEPAD, personal communication, 2002).

Table 3.3 Volumes of substances (excluding ethoxylates) produced from alkylphenols

Substance	Volumes in Western Europe (tonnes/year)					
	Hydrogenation++	Lubricant additives	Phenolic oximes	Phenolic resins	Plastic additives	Poly-carbonate
Nonylphenol (1997 data)	0	0	2,500	22,500	1,000	0
Other Alkylphenols (1999 data)						
4-*tert*-Butylphenol	2,500	2,500	0	8,000	500	5,000
4-*tert*-Pentylphenol	0	0	0	400	0	0
4-*tert*-Octylphenol*	0	0	0	22,458	220	0
2,4-Di-*tert*-butylphenol	0	0	0	0	13,000	0
2,6-Di-*tert*-butylphenol	0	0	0	0	15,000	0
Phenol, styrenated	0	0	0	1,600	0	2000
Dodecylphenol, branched*	0	Major use#	0	Minor use#	0	

* Data for 2001

++ Hydrogenation: reaction with hydrogen under pressure and with a catalyst to produce 4-*tert*-butylcyclohexan-1-ol

\# actual values considered confidential

On the basis of the data presented by CEPAD it is clear that, although the total quantities of alkylphenols and nonylphenol produced are similar, their use patterns are markedly different. Whereas 59.9 per cent of nonylphenol was used in the production of nonylphenol ethoxylates (based on data in the risk assessment for 1997), only 1.4 per cent of the other alkylphenols (for example 4-*tert*-octylphenol) are used in this way. In contrast, the other alkylphenols are mainly used to produce lubricant additives (25.9 per cent of total), phenolic resins (23.8 per cent) and plastic additives (35.1 per cent).

Information from IUCLID on the shorter chain alkylphenols (methylphenols, dimethylphenols and trimethylphenols) indicates that these are primarily used as intermediates in chemical synthesis and not in the production of ethoxylate

surfactants. Methylphenols and dimethylphenols are also used in the paints, lacquers and varnishes industry.

3.3 Physicochemical properties

The physical behaviour of the alkylphenols influences the process used to make other products, and the nature of those products themselves. For example, short chain alkylphenols such as methylphenol, dimethylphenol and trimethylphenol would produce ethoxylates that would perform poorly as surfactants, since the alkyl chain is too short to impart sufficient hydrophobicity to the molecule. Detailed consideration of these as substances for use in nonylphenol ethoxylate substitution has not been taken any further. CEPAD indicated that the same was also true for the butylphenols. These issues are summarised in Table 3.4.

For the plastics, resins and stabiliser uses, much depends on the type and use of the end product as this will determine the physicochemical properties required from the alkylphenol. However, few substitutes are likely based on these physicochemical requirements. Long chain alcohols are not suitable as substitutes for the resins, and no suitable compounds have been identified by industry for production of tris(4-nonylphenyl)phosphite (TNPP).

Table 3.4 Summary of the problems of using alkylphenols as substitutes for nonylphenol to produce ethoxylate surfactants

Substance	Physical behaviour	Price of feedstock
2-*tert*-Butylphenol	The short C_4 alkyl chain means the substance is unsuitable for use as a surfactant	Price is significantly higher than for nonylphenol
4-*tert*-Butylphenol		
4-*tert*-Pentyl-phenol	There are problems with the availability of the feedstock; the short C_5 alkyl chain means the substance is unsuitable for use as a surfactant	Price is significantly higher than for nonylphenol
4-*tert*-Octylphenol	There are handling problems since it is solid at room temperature (nonylphenol is a viscous liquid)	Price is significantly higher (80–100%) than for nonylphenol
2,4-Di-*tert*-butyl-phenol	The ethoxylates produced have nearly no surface active properties and are unsuitable for use as a surfactant	Price is significantly higher than for nonylphenol
2,6-Di-*tert*-butyl-phenol	The ethoxylates produced have nearly no surface active properties and are unsuitable for use as a surfactant	Price is significantly higher (200–300%) than for nonylphenol
Dodecylphenol	The C_{12} alkyl chain means that resulting surfactants will have poor performance characteristics for most uses	Price is significantly higher than for nonylphenol

3.4 Economic and other factors

The price differential between candidate alkylphenols and nonylphenol is an important factor to consider. It is affected by feedstock price, changes in processing requirements and final product performance (including reformulation). Phenol/formaldehyde resins in particular are normally very specific products; small changes in the production process and/or substitution of individual components may have a major impact on the properties of the end product.

Tables 3.4 and 3.5 summarise the information presented by CEPAD for some of the identified alkylphenols in relation to the main uses of nonylphenol. It is apparent that there are problems with the use of all these materials as substitutes for nonylphenol, which arise from both the performance of the resulting products and the price of the alkylphenols themselves (relative to nonylphenol). However, it should be recognised that cost issues for the production of alkylphenol substitutes for nonylphenol may change if there was a wider market for these materials as substitutes. It is also known that both 4-*tert*-octylphenol and dodecylphenol (branched) are currently used to make ethoxylates and phenol/formaldehyde resins.

Table 3.5 Summary of the problems of using alkylphenols as substitutes for nonylphenol for production of resins, plastics, stabilisers, etc.

Use	Possible AP substitute	Problems with use of alkylphenols as substitutes
Production of phenol/ formaldehyde resins	4-*tert*-Butylphenol	Price is significantly higher (80–100%) than for nonylphenol; the performance of the resins in the intended end-uses is not acceptable
	4-*tert*-Pentylphenol	
	4-*tert*-Octylphenol	
	4-Cumylphenol (not an alkylphenol)	
	Dodecylphenol	Price is significantly higher (80–100%) than for nonylphenol
Catalyst in the curing of epoxy resins	None, perhaps dodecylphenol	The curing performance is poor
Intermediate in the production of other plastic stabilisers	4-*tert*-Butylphenol	Price is significantly higher (200–300%) than for nonylphenol
	2,4-di-*tert*-Butylphenol	Price is significantly higher (200–300%) than for nonylphenol
	2,6-di-*tert*-Butylphenol	Price is significantly higher (200–300%) than for nonylphenol

3.5 Environmental concentrations

3.5.1 Releases to the aquatic environment

Relative to other individual alkylphenols there is a greater production volume of nonylphenol and nonylphenol ethoxylates. As a result their releases to the aquatic environment are currently larger with consequent implications for environmental concentrations. For example, in England and Wales, total emissions from Part A Integrated Pollution Control (IPC) processes in 1998 were 6,065 kg for nonylphenol (6,000 kg to controlled waters and 65 kg to sewers) and 34,200 kg for nonylphenol ethoxylates (18,500 kg to controlled waters and 15,700 kg to sewers). In contrast, only 300 kg of octylphenols were released, all to controlled waters. No data were available for other alkylphenols (Environment Agency, 1999).

3.5.2 Monitoring data

There are limited monitoring data for the candidate alkylphenols. Most of the available data from recent years is for nonylphenol and its ethoxylates. Table 3.6 summarises data obtained from the European Environment Agency and from CEPAD on the levels of a number of these alkylphenols (and nonylphenols) in the River Elbe in Germany.

The majority of these data are for 4-*tert*-octylphenol and indicate that European riverine and estuarine surface water concentrations in the period covered (1994–1998) were generally below 1 μg/l. The levels of octylphenol ethoxylates measured in surface waters on the Elbe catchment were below 10 ng/l on all occasions. The levels of butylphenol and pentylphenol measured in surface water samples were generally extremely low: below 10 and 2 ng/l, respectively.

In contrast, while dissolved concentrations of nonylphenols in surface waters are generally below 1 μg/l, elevated concentrations are found at locations receiving discharges from industrial plants or sewage treatment works (STW).

Levels of alkylphenols (other than nonylphenol) measured in effluent discharges were also generally lower than those for nonylphenol. Blackburn and Waldock (1995) measured the levels of octylphenols in discharges from 15 sewage treatment works effluents and the concentrations were generally below 1 μg/l, although values of up to 2.3 μg/l were measured in works discharging to the River Lea. Measured concentrations of octylphenol mono- and diethoxylate were higher at between <7.3 and 22 μg/l. In contrast, the total extractable concentrations of nonylphenol measured in sewage treatment works discharges varied from 0.2–0.9 μg/l at plants receiving mainly domestic wastes and operating secondary treatment, to 6.7 μg/l at a plant receiving mainly domestic wastes and operating primary treatment and to 330 μg/l at a plant receiving wastes from an industrial area.

Table 3.6 Summary of surface water monitoring data for alkylphenols (as dissolved concentrations)

Alkylphenol	Data source				
	Country	Location	Year	Concentration (μg/l)	Ref.
Butylphenols	England	6 Rivers[a]	1994	<0.05	1
		6 Estuaries[b]	1994	<0.05	1
	Germany	4 Rivers[c]	1998	<0.01 (1 value = 0.078)	2
Pentylphenol	Germany	4 Rivers[c]	1998	<0.0002	2
Octylphenols	England	6 Rivers[a]	1994	<1	1
		1 Canal[e]	1999	<0.4	
		6 Estuaries[b]	1994 1999	<1 <0.25	1, 5
	Scotland	4 Rivers[d]	1996	<3	3
	Denmark	Unknown	1997	<0.2	4
	Germany	4 Rivers[c]	1998	<0.01	2
Nonylphenol	England	6 Rivers[a]	1994	<0.2–53.0	1
		6 Estuaries[b]	1994	<0.08–3.1	1
	Scotland	4 Rivers[d]	1996	<2	3
	Denmark	Unknown	1997	<0.12	4
	Germany	4 Rivers[c]	1998	<0.02–0.21	2

Key:

[a] Rivers Aire, Arun, Great Ouse, Lea, Thames, Wye
[b] Blyth, Mersey, Tees, Wear and Wyre Estuaries, Poole Harbour and Southampton Water
[c] Rivers Elbe, Mulde, Saale and Schwarzer Elster
[d] Rivers Almond and Blackcart, South Quiech and Annick Water
[e] Manchester Ship Canal.
1, Blackburn and Waldock (1995); 2, Working Group for the Cleanliness of the Elbe (1998); 3, SEPA (1997); 4, Danish Ministry of the Environment (1997); 5, Environment Agency, UK (NCEDS, 1999)

In the UK, the Environment Agency North West region (NCEDS, 1999) carried out monitoring for 4-*tert*-octylphenol over a period of several months on the trade effluent from a production plant, the effluent from a sewage treatment plant and receiving waters on the Wyre peninsula. In all of the STW effluent samples (n=21) the 4-*tert*-octylphenol concentration was below the limit of detection (200 or 1000 ng/l). SEPA (1997) found that levels of nonylphenols discharged from seven sewage treatment works varied from < 0.4 to 12.9 μg/l, whereas levels of 4-*tert*-octylphenol were generally < 3.3 μg/l.

The study on the Elbe catchment also measured levels of alkylphenols (and certain ethoxylates) in sediment samples (see Table 3.7). The data indicated that the levels of nonylphenol and nonylphenol ethoxylates were an order of magnitude higher than those of butylphenol, pentylphenol and 4-*tert*-octylphenol and its ethoxylates.

Table 3.7 Summary of data on alkylphenol (and ethoxylate) concentrations in River Elbe catchment sediments

Substance	Concentration range (ng/g dry weight) in River Elbe catchment sediments
Butylphenol	19–93
Pentylphenol	17–96
4-*tert*-Octylphenol	21–116
Octylphenol monoethoxylate (OP1EO)	30–113
Octylphenol diethoxylate (OP2EO)	45–140
Nonylphenol	367–1378
Nonylphenol monoethoxylate (NP1EO)	323–1027
Nonylphenol diethoxylate (NP2EO)	546–1797

Concentrations of 4-*tert*-octylphenol have been reported in samples of two types of freshwater fish collected between 1992 and 1997 from several German rivers (UBA, 1999). Measured concentrations were generally above the limit of detection of 0.2 μg/kg wet weight; the highest reported level was 5.5 μg/kg wet weight. 4-*tert*-Octylphenol has also been reported in a marine alga (*Fucus vesiculosus*), a marine invertebrate (*Mytilus edulis*) and two types of marine fish from Germany (UBA, 1999) for samples collected between 1985 and 1996 at several locations. Measured concentrations were generally below or slightly above the limit of detection of 0.2 μg/kg wet weight; the highest reported level was 1.1 μg/kg.

CEPAD has commented that the presence of low levels of butylphenol, pentylphenol and octylphenol in receiving water samples (alongside elevated levels of nonylphenol) is possibly a consequence of the presence of low levels of these substances as impurities of nonylphenol. Nonylphenol is produced using technical grade nonane which can typically contain 1–5 per cent octane, 1 per cent butane and 1 per cent pentane.

3.6 Persistence

There are few reliable data on the persistence of alkylphenols in the environment. Alkylphenols would not be expected to be susceptible to hydrolysis in the aquatic environment, but are susceptible to indirect photolysis by hydroxyl radicals in the atmosphere. The half-lives estimated for most alkylphenols in the atmosphere are of the order of a few hours.

Information on biodegradation has been located for only a few of the identified compounds considered in this review. Many of these originate from a secondary data source such as the non-confidential IUCLID so the validity has not been checked. However, there are many naturally produced alkylphenolic compounds and it is expected that micro-organisms would have developed enzymes capable of degrading alkylphenols. The available biodegradation data suggests that this is true: many of the alkylphenols are

readily biodegradable and many of the others are inherently biodegradable. The least biodegradable appear to be those substances with single branched alkyl chains of C_5 or longer or with more than one branched alkyl chain. Table 3.11 provides a summary of the available data for all identified alkylphenols.

There are a number of substances in Table 3.11 for which no experimental biodegradation data are available. For these substances, the probable biodegradation rate (in terms of whether ultimate biodegradation (mineralisation) is likely to occur over timeframes of the order of days, weeks, months or years) has been estimated using the Syracuse Research Corporation BIOWIN (v3.63) program. It is recognised that estimation methods for biodegradation are less well developed and less reliable than estimation methods commonly used for other environmentally relevant properties (such as log octanol-water partition coefficient, K_{ow} and acute toxicity to aquatic organisms). In order to take this into account here, biodegradation predictions have also been carried out for the alkylphenols where the biodegradation behaviour has been determined experimentally (the predictions for these substances are also included in Table 3.11). This provides some check on how well the predictions compare with the actual biodegradation behaviour for this group of substances. When compared in this way, it can be seen that, although the correlation is not high, the predictions for many of the substances that are known to be readily biodegradable give an ultimate biodegradation timeframe of weeks. For many of the substances that are known to be inherently biodegradable, or of low biodegradability, the predictions indicate an ultimate biodegradation timeframe of weeks to months or longer.

3.7 Bioaccumulation

There are few reliable data on the potential for bioaccumulation of alkylphenols. Bioconcentration factor (BCF) values have been located for only a few of the compounds considered in this review. Many of these originate from a secondary data source such as the non-confidential IUCLID so the validity has not been checked. It is therefore not surprising that there is a wide range of values, ranging from 37 (2,6-dimethylphenol and 4-*sec*-butylphenol) to 23,200 (2,4,6-tris(1,1-dimethyl ethyl) phenol). The majority of the alkylphenols for which data are available, however, appear to display a low to moderate potential to bioaccumulate in tissues with BCFs below 1,000. Table 3.11 provides a summary of the available data for all identified alkylphenols.

For several substances, no measured BCF value is available. In these cases, an estimate of the BCF has been obtained using the following equations recommended in the EU technical guidance document (TGD) for risk assessment of industrial chemicals (TGD, 2003).

For $\log K_{ow} \leq 6$ $\quad \log BCF = 0.85 \times \log K_{ow} - 0.70$

For $\log K_{ow} > 6$ $\quad \log BCF = -0.20 \times (\log K_{ow})^2 + 2.74 \times \log K_{ow} - 4.72$

The BCF values estimated in this way are included in Table 3.11. The values obtained from these equations have an uncertainty attached to them. For

those alklyphenols where measured BCF values are available, the correlation with log K_{ow} is not good, and the real BCF value tends to be overestimated when the log K_{ow} is high. This is probably due to rapid biotransformation and excretion, which is likely to apply for the simpler compounds at least. It should also be noted that the estimation method depends on the log K_{ow}. For some substances a measured value was not available, and for these, a log K_{ow} was estimated from chemical structure using the Syracuse Research Corporation Log K_{ow} (v1.60) program. These data are also reported in Table 3.11 and it should be noted that this adds a further degree of uncertainty to the estimated BCF for these substances.

3.8 Ecotoxicity data

3.8.1 General toxicity

Data incorporated in the summary datasheets (see Annex I) were obtained from the sources outlined in Section 1.2. There is considerable variability in the amount of data available. There is no information on toxicity to terrestrial organisms for any of the substances (other than nonylphenol). Mammalian toxicity has not been considered in this report, since effects on the aquatic environment appear more significant for this class of substances.

Only three alkylphenols (other than nonylphenol) appear to have valid short-term toxicity data available for freshwater fish, invertebrates and green algae (representing an aquatic food chain, and generally considered as a minimum data set for predicting environmental toxicity). These are 4-*tert*-butylphenol, 4-*tert*-octylphenol and dodecylphenol. The data are summarised in Table 3.8 along with that for nonylphenol. The data for 4-*tert*-butylphenol were taken from Waern (2000) and OECD SIDS documents (SIDS, 2000), but since they are currently being assessed in depth by Norway under the Existing Substances Regulation they are not discussed in any detail. The data for 4-*tert*-octylphenol and dodecylphenol are discussed and referenced in full in separate draft risk assessment reports (Environment Agency, 2003a and 2003b). The data for nonylphenol are taken from the published risk assessment (ECB, 1999).

Table 3.8 clearly shows that the sensitivity of a range of organisms to 4-*tert*-octylphenol is similar to that found for nonylphenol. For many species, concentrations causing particular effects are the same within a factor of three. However, there is a difference in the algal toxicity data, and there is no information about chronic toxicity to mysids. There is also some evidence that endocrine-mediated effects may occur at lower concentrations (see section 3.8.2).

While far fewer and less certain data are available for dodecylphenol, the toxicity profile is again very similar to nonylphenol (although there is still a difference in the algal toxicity data). 4-*tert*-Butylphenol shows a 10- to 100-fold reduction in sensitivity compared with nonylphenol.

Table 3.8 Comparison of the lowest reliable acute and chronic toxicity data for four data rich alkylphenols (units are μg/l; data are considered valid unless identified as 'use with care')

Data type	4-*tert*-Butylphenol (C_4)	4-*tert*-Octylphenol (C_8)	Nonylphenol (C_9)	Dodecylphenol, branched (C_{12})
Log K_{ow}	3.3	4.12	4.48	5.5
Fish				
Acute (freshwater) 96-h LC_{50}	5,100 (Medaka, *Oryzias latipes)*	250 (Fathead minnow *Pimephales promelas*) 170 (6-d LC_{50} Rainbow trout *Oncorhynchus mykiss*)	128 (Fathead minnow *Pimephales promelas*)	140 (use with care, Atlantic salmon *Salmo salar*) $\geq$500 (96-h NOEC Golden orfe *Leucuscus idus*)
Acute (saltwater) 96-h LC_{50}	-	280–340 (use with care, Mummichog *Fundulus heteroclitus*)	310 (Sheepshead minnow *Cyprinodon variegatus*)	-
Chronic (freshwater)	-	6.1 (60-day early life stage $NOEC_{growth}$ Rainbow trout *Oncorhynchus mykiss*)	7.4 (33-day $NOEC_{survival}$ Fathead minnow *Pimephales promelas*)	-

Table continued overleaf

Table 3.8 continued

Data type	4-*tert*-Butylphenol (C_4)	4-*tert*-Octylphenol (C_8)	Nonylphenol (C_9)	Dodecylphenol, branched (C_{12})
Invertebrates				
Acute (freshwater) 48-h EC_{50} *Daphnia magna*	3,400-3,900	270	85	93
Acute (freshwater) 96-h EC_{50} *Gammarus pulex*	-	13.3	12.7 (use with care)	-
Acute (saltwater) 96-h LC_{50} *Crangon septemspinosa*	-	1,100 (use with care)	300 (use with care)	150 (use with care)
Acute (saltwater) 96-h E(L)C_{50} *Mysidopsis bahia*	-	53.4	43	-
Chronic (freshwater) 21-day NOEC *Daphnia magna*	730	62 (surviving offspring)	24	-
Chronic (saltwater) 28-day NOEC *Mysidopsis bahia*	-	-	3.9	-

Table continued overleaf

Table 3.8 continued

Data type	4-*tert*-Butylphenol (C_4)	4-*tert*-Octylphenol (C_8)	Nonylphenol (C_9)	Dodecylphenol, branched (C_{12})
Algae				
Acute (freshwater) 72-h EC_{50} (growth rate) *Scenedesmus subspicatus*	11,000	1,100 (use with care)	323 (or 1300 use with care)	>770
Acute (saltwater) 96-h EC_{50} cell growth *Skeletonema costatum*	-	-	27	-
Chronic (freshwater) 72-h EC_{10} (growth rate) *Scenedesmus subspicatus*	-	300 (use with care)	25.1 (or 500 use with care)	>770 (NOEC = 440)

No other alkylphenols appear to have a basic data set available. However, in some studies a range of alkylphenols was tested with the same species, thereby allowing conclusions to be drawn regarding the effects of chain length (and octanol-water partition coefficient, K_{ow}) on toxicity. These are discussed below.

Gerritsen *et al*. (1998) assessed the toxicity of a range of alkylphenols to young (<24-h old) *Daphnia magna*, using the no observed effect concentration (NOEC) calculated from 96-hour survival studies as the endpoint. There was a marked reduction in NOEC value with increasing alkylphenol chain length (and thus increasing K_{ow} values) (see Table 3.9).

Table 3.9 Summary of 96-h NOECs of alkylphenols for mortality of juvenile *Daphnia magna*

Substance	No effect concentration (mg/l)
4-*sec*-Butylphenol	9.7
4-*tert*-Butylphenol	8.6
4-*tert*-Pentylphenol	1.8
4-*tert*-Octylphenol	0.19
4-Nonylphenol	0.3
2,4-Di-*tert*-butylphenol	0.85

McLeese *et al*. (1981) assessed the toxicity of a range of alkylphenols to the marine shrimp *Crangon septemspinosa* in 96-hour static tests (at 10°C) using mortality as the endpoint. The long chain alkylphenols were more toxic than the short chain alkylphenols (see Table 3.10). The data also suggest that there can be variability in the toxicity of different isomers, with a range of 96-hour LC_{50} values of 1.3–5.2 mg/l for butylphenol for example. The study is not considered to be fully valid, and so the data are not necessarily comparable with other valid study results for the same species. The variation in the sequence was not given any discussion by the study authors.

Table 3.10 Summary of concentrations of alkylphenols causing mortality of *Crangon septemspinosa*

Substance	96-h LC_{50} (mg/l)
o-*sec*-Butylphenol	1.3
p-*sec*-Butylphenol	1.8
o-*tert*-Butylphenol	2.4
m-*tert*-Butylphenol	5.2
p-*tert*-Pentylphenol	1.7
p-Hexylphenol	0.9
p-Heptylphenol	0.6
p-*tert*-Octylphenol	1.1
p-Nonylphenol	0.3
p-Dodecylphenol	0.15

Other recent comparative data have indicated that the copepod *Acartia tonsa* is more sensitive to para-substituted alkyphenols than to other alkyl substitutions (Buffagni *et al*., 2001). The same source also suggested that test

results using a mixture of alkylphenols might have resulted in some synergistic effects on the organisms.

Summary

Overall, the general toxicity data indicate that aquatic organisms appear more sensitive to the longer chain alkylphenols (such as dodecylphenol, 4-*tert*-octylphenol and nonylphenol) than the shorter chain alkylphenols (such as 4-*tert*-butylphenol). This is to be expected in view of the change in partitioning behaviour as the alkyl chain length increases (for example as modelled by the n-octanol-water partitioning coefficient). However, the longer chain alkylphenols appear to exhibit similar toxicities.

The available aquatic toxicity data for the alkylphenols considered in this study are summarised in Table 3.11. For several substances, no experimental data are available for either the acute or chronic endpoints. In these cases, values have been estimated using the Scyracuse Research Corporation ECOSAR Program (v0.99b). This program predicts the toxicity for fish, *Daphnia* and algae from chemical structure using methods applicable to phenolic chemicals as a group. It should be noted that there are some uncertainties attached to these values.

3.8.2 Endocrine disruption

Alkylphenols such as nonylphenol are now known to affect the endocrine system, by acting as weak oestrogens. The key data currently required to determine whether any substance can be considered to cause endocrine mediated responses are longer-term *in vivo* assays (such as multi-generational tests) or those where exposure is targeted towards critical windows of sensitivity in the life history of the organism. The endpoints of greatest significance are those which are associated with reproduction and/or development. For non-standard protocol endpoints, including *in vivo* screening studies, the assessment of endpoint relevance is usually a subjective decision based on expert judgement. While robust *in vitro* data are useful in making judgements about the presumption of hazard they are not currently linked directly to, or are predictive of, adverse toxicological effects associated with endocrine disruption.

The most extensive data set available (other than for nonylphenol) is for 4-*tert*-octylphenol. These data are considered in detail in the draft Environment Agency risk assessment report for that substance (Environment Agency, 2003a). There are some indications that molluscs could be more sensitive than fish or other invertebrates. Comparable data for nonylphenol on endocrine-mediated effects in molluscs did not exist at the time the assessment for that substance was completed (1999). 4-*tert*-Pentylphenol can also induce oviduct formation in male fish (Gimeno *et al.,* 1996), and so it is likely that many 4-alkylphenols have the potential to act as weak oestrogens.

No other *in vivo* aquatic data have been found for any other alkylphenol. Recently the Chemicals Evaluation and Research Institute in Japan (CERI,

2001) developed a competitive binding assay for the medaka (*Oryzias latipes*) oestrogen receptor α and have used the assay to measure the relative binding affinity of a number of alkylphenols. The substances tested were linear and branched chain butyl-, pentyl- and octylphenol, and a mixture of nonylphenol isomers. The linear compounds bound to the receptor in the same manner but with low binding affinity relative to that of 17β-oestradiol. Linear 4-octylphenol had the highest relative binding affinity (RBA) of 0.077 in the set compared with 100 for 17β-oestradiol. However, alkylphenols with branched chains exhibited relatively higher affinities than those of the linear compounds and branched 4-octylphenol had the highest RBA value of these. The other values for the branched substances were:

- nonylphenol: 7.5
- 4-pentylphenol: 1.1
- 4-butylphenol: 0.15.

In this study binding affinity with the medaka oestrogen receptor appears to be related to the structure of the isomer and the length of the alkyl chain; the longer chain branched substances have the highest affinity. The nonylphenol results do not appear to support this completely, but since a mixture of isomers was tested comparison with the other results (linear versus branched) is difficult. The results of this study indicate that the structure and conformation of the alkylphenol is important in determining the degree of binding to this steroid receptor, although this does not provide any indication of the relative potency or activity of the substance on binding.

3.9 PBT assessment

The EU TGD gives criteria for defining a persistent (P), bioaccumulative (B) and toxic (T) substance in relation to the marine environment (TGD, 2003). The alkylphenols considered in this assessment have been considered against these screening criteria and the findings are summarised in Table 3.11.

In relation to the persistence criterion, only substances that are readily biodegradable (or have a predicted ultimate biodegradation timeframe of weeks; see Section 3.6) have been assumed not to be potentially persistent (P) or very persistent (vP). It should be noted that, in general, actual biodegradation simulation tests would be necessary to determine if these substances do in fact meet the P or vP criteria.

3.10 Summary of fate and effect data

Table 3.11 summarises the available fate and effect data for all the alkylphenols that have been considered in this report. Individual data sheets with additional details are provided in Annexes I and II. Water solubility data are expressed at 25°C unless stated otherwise.

Table 3.11 Summary fate and hazard data on identified alkylphenols

Substance	CAS No.	Formula	Water Solubility	Log K_{ow}	Biodegradation	BCF	Lowest aquatic toxicity values (mg/l)		PBT?	Reference	Comment
							Acute	Chronic			
Methylphenols	1319-77-3	C_7H_8O	25 g/l	2.1[a]	Readily biodegradable (biodegrades in weeks[b])	12[c]	7	0.12[a]	No	IUCLID	Log K_{ow}, BCF and chronic toxicity estimated
2-Methylphenol	95-48-7	C_7H_8O	26 g/l	1.95; 2	Readily biodegradable (biodegrades in weeks[b])	10[c]	2	11	No	IUCLID	BCF estimated
3-Methylphenol	108-39-4	C_7H_8O	24 g/l	1.96; 2–2.15	Readily biodegradable (biodegrades in weeks[b])	4,900	6	10	No	IUCLID	The BCF seems high given the log K_{ow}
4-Methylphenol	106-44-5	C_7H_8O	19.4 g/l at 20°C	1.94	Readily biodegradable (biodegrades in weeks[b])	8.9[c]	7.5	1.5–2.6	No	IUCLID	BCF estimated
2,6-Dimethyl-phenol	576-26-1	$C_8H_{10}O$	5.9 g/l	2.36	Readily biodegradable (biodegrades in weeks[b])	37	11.2	0.078[a]	No	IUCLID	Chronic toxicity estimated

Table continued overleaf

Table 3.11 continued

Substance	CAS No.	Formula	Water Solubility	Log K_{ow}	Biodegradation	BCF	Lowest aquatic toxicity values (mg/l)		PBT?	Reference	Comment
							Acute	Chronic			
Dimethylphenols	1300-71-6	$C_8H_{10}O$	Slightly soluble	2.6[a]	Biodegrades in weeks[b]	32[c]	3.7[a]	0.078[a]	No	IUCLID	Solubility data – descriptor only, log K_{ow}, biodegradation, BCF and aquatic toxicity estimated
3,5-Dimethyl-phenol	108-68-9	$C_8H_{10}O$	4.8–5.3g/l	2.06–2.55	Readily biodegradable (biodegrades in weeks[b])	11–29[c]	10–35	0.078[a]	No	IUCLID	BCF and chronic toxicity estimated
2-Ethylphenol	90-00-6	$C_8H_{10}O$	0.01g/l at 22°C	2.47	Inherently biodegradable (biodegrades in weeks[b])	44	3.9[a]	0.083[a]	No	ChemFinder, TOXNET, SRC PhysProp Database	Biodegradation information very limited, aquatic toxicity estimated
4-Ethylphenol	123-07-9	$C_8H_{10}O$	4.9 g/l	2.58	Inherently biodegradable (biodegrades in weeks[b])	54	5.7	63.5	No	ECOTOX, SRC PhysProp Database	Biodegradation information very limited

Table continued overleaf

Table 3.11 continued

Substance	CAS No.	Formula	Water Solubility	Log K_{ow}	Biodegradation	BCF	Lowest aquatic toxicity values (mg/l)		PBT?	Reference	Comment
							Acute	Chronic			
2-Isopropyl-phenol	88-69-7	$C_9H_{12}O$	1.15 g/l	2.88	Biodegrades in weeks[b]	56[c]	2.9[a]	0.060[a]	No	SRC PhysProp Database	Biodegradation, BCF and aquatic toxicity estimated
2,3,6-Trimethyl-phenol	2416-94-6	$C_9H_{12}O$	1.42; 1.58 mg/l	2.72	Readily biodegradable (biodegrades in weeks–months[b])	41[c]	8.2	0.050[a]	No	IUCLID; USEPA (2001)	BCF and chronic toxicity estimated
2-*tert*-Butyl-phenol	88-18-6	$C_{10}H_{14}O$	700 mg/l; 394 mg/l; 2.3 g/l at 20°C	2.7–3.5	Readily biodegradable (Hüls study) (biodegrades in weeks–months[b])	39–188[c]	2.4	0.042[a]	No	ChemFinder; SRC PhysProp Database; McLeese *et al.* (1981); BUA (2001); USEPA (2001); SASOL (2001)	Further data available in German BUA report (2001). BCF and chronic toxicity estimated

Table continued overleaf

Table 3.11 continued

Substance	CAS No.	Formula	Water Solubility	Log K_{ow}	Biodegradation	BCF	Lowest aquatic toxicity values (mg/l)		PBT?	Reference	Comment
							Acute	Chronic			
3-*tert*-Butyl-phenol	585-34-2	$C_{10}H_{14}O$	2,067 mg/l	2.6; 3.3	Biodegrades in weeks–months[b]	32[c]; 127[c]	5.2	0.042[a]	No	Chem Finder; SRC PhysProp Database	Not commercially available, biodegradation, BCF and chronic toxicity estimated
4-*tert*-Butyl-phenol	98-54-4	$C_{10}H_{14}O$	610 mg/l ; 800 mg/l at 20°C; 500 mg/l	3.29	Readily biodegradable (biodegrades in weeks–months[b])	120	3.4–3.9	0.73	No	Non-confidential IUCLID; Waern (2000); SIDS (2000); USEPA (2001); SASOL (2001); KEMI (2000)	A full ESR assessment is under way, with Norway as the rapporteur
2-*sec*-Butyl-phenol	89-72-5	$C_{10}H_{14}O$	1,659 mg/l; 319 mg/l	2.8; 3.27; 3.46	Biodegrades in weeks[b]	48[c], 120[c], 174[c]	1.3	0.040[a]	No	ChemFinder; SRC PhysProp Database	Biodegradation, BCF and chronic toxicity estimated

Table continued overleaf

Table 3.11 continued

Substance	CAS No.	Formula	Water Solubility	Log K_{ow}	Biodegradation	BCF	Lowest aquatic toxicity values (mg/l)		PBT?	Reference	Comment
							Acute	Chronic			
4-*sec*-Butyl-phenol	99-71-8	$C_{10}H_{14}O$	960 mg/l	2.1; 3.08; 3.46	Biodegrades in weeks[b]	37	0.74	0.040[a]	No	SRC PhysProp Database; McLeese *et al.* (1981); Gerritsen *et al.* (1998)	Not commercially available, biodegradation and chronic toxicity estimated
2-*tert*-Pentyl-phenol	3279-27-4	$C_{11}H_{16}O$	113 mg/l[a]	3.9[a]	Biodegrades in weeks–months[b]	412[c]	1.4[a]	0.027[a]	No	SDS	All data estimated
4-*tert*-Pentyl-phenol	80-46-6	$C_{11}H_{16}O$	168 mg/l; 37 mg/l at 20°C	2.1; 4.03	Not readily biodegradable (biodegrades in weeks–months[b])	12[c]; 531[c]	1.7	0.063	No	ChemFinder; NTP; McLeese *et al.* (1981); SASOL (2001)	BCF estimated
2-*tert*-Butyl-p-methylphenol	2409-55-4	$C_{11}H_{16}O$	101mg/l[a]	4.0[a]	Biodegrades in weeks–months[b]	501[c]	1.4[a]	0.026[a]	No	IUCLID (confidential); IUCLID non-confidential	All data estimated

Table continued overleaf

Table 3.11 continued

Substance	CAS No.	Formula	Water Solubility	Log K_{ow}	Biodegradation	BCF	Lowest aquatic toxicity values (mg/l)		PBT?	Reference	Comment
							Acute	Chronic			
4-Hexylphenol	2446-69-7	$C_{12}H_{18}O$	30 mg/l[a]	3.6	Biodegrades in weeks[b]	229[c]	0.19	0.016	No	McLeese *et al.* (1981)	Not commercially available, water solubility, biodegradation, BCF and chronic toxicity estimated
2-Cyclohexyl-phenol	119-42-6	$C_{12}H_{18}O$	44 mg/l[a]	4.3[a]	Biodegrades in weeks[b]	902[c]	0.95	0.019	No		Production levels uncertain, all data estimated
2-*tert*-Butyl-4-ethylphenol	96-70-8	$C_{12}H_{18}O$	33.1 mg/l	4.46	Biodegrades in weeks–months[b]	1,233[c]	0.81	0.017	No	SRC PhysProp Database	Biodegradation, BCF and aquatic toxicity estimated

Table continued overleaf

Table 3.11 continued

Substance	CAS No.	Formula	Water Solubility	Log K_{ow}	Biodegradation	BCF	Lowest aquatic toxicity values (mg/l)		PBT?	Reference	Comment
							Acute	Chronic			
4-Heptylphenol	1987-50-4	$C_{13}H_{20}O$	9.6 mg/l[a]	5.0[a]	Biodegrades in weeks[b]	3,548[c]	0.6	0.010	No	ECOTOX	Not commercially available, water solubility, logK_{ow}, biodegradation, BCF and chronic toxicity estimated. Not PBT by analogy with octylphenol (BCF likely to be lower)
Octylphenols	27193-28-8	$C_{14}H_{22}O$	See below							Confidential IUCLID	Not of commercial relevance
4-Octylphenol	1806-26-4	$C_{14}H_{22}O$	See below								
4-*tert*-Octyl-phenol	140-66-9	$C_{14}H_{22}O$	12.6 mg/l at 20.5°C; 17–19 mg/l at 22°C	4.12	Not readily biodegradable (biodegrades in weeks–months[b])	634	0.013	0.006	No	Environment Agency (2003a)	This is the only octylphenol that is commercially available

Table continued overleaf

Table 3.11 continued

Substance	CAS No.	Formula	Water Solubility	Log K_{ow}	Biodegradation	BCF	Lowest aquatic toxicity values (mg/l)		PBT?	Reference	Comment
							Acute	Chronic			
Isooctylphenol	11081-15-5	$C_{14}H_{22}O$	See comments (no data available)								Production was terminated in 1994
2,4-Di-*tert*-butylphenol	96-76-4	$C_{14}H_{22}O$	12 mg/l at 20°C	5.19	Not readily biodegradable (biodegrades in weeks–months[b])	~660 (see note)	1.8	0.008[a]	No	SDS; HSDB; IUCLID (non-confidential); USEPA (2001)	BCF and chronic toxicity estimated. BCF derived from log K_{ow} (5,146) likely to be too high by analogy with next substance
2,6-Di-*tert*-butylphenol	128-39-2	$C_{14}H_{22}O$	4.11 mg/l at pH 7	4.92	Not readily biodegradable (biodegrades in weeks–months[b])	660	0.076	0.019[a]	No	HSDB; SIDS Initial Assessment profile	Chronic toxicity estimated
2,4-Di-*tert*-pentylphenol	120-95-6	$C_{16}H_{26}O$	0.015 g/l at 20°C; 0.44 mg/l	6.31	Not readily biodegradable (biodegrades in weeks–months[b])	40,381[c]	1–10 mg/l	0.003[a]	Maybe	SDS; SASOL (2001); USEPA (2001)	BCF and chronic toxicity estimated

Table continued overleaf

Table 3.11 continued

Substance	CAS No.	Formula	Water Solubility	Log K_{ow}	Biodegradation	BCF	Lowest aquatic toxicity values (mg/l)		PBT?	Reference	Comment
							Acute	Chronic			
2,6-Di-*tert*-butyl-4-ethylphenol	4130-42-1	$C_{16}H_{26}O$	2 mg/l[a]	5.52	Biodegrades in months[b]	9,817[c]	0.23[a]	0.007[a]	Maybe	SRC PhysProp Database	Water solubility, biodegradation, BCF and aquatic toxicity estimated
Dodecylphenol, mixed isomers	27193-86-8	$C_{18}H_{30}O$	See below								Preferred CAS No. is 74499-35-7 or 121158-58-5
4-Dodecylphenol	104-43-8	$C_{18}H_{30}O$									
Isododecylphenol	11067-80-4	$C_{18}H_{30}O$									
Phenol, (tetrapropenyl) derivatives and dodecylphenol, branched	74499-35-7 and 121158-58-5	$C_{18}H_{30}O$	54 µg/l at 20°C	5.5	Not readily biodegradable	9,440	0.093	No data available	Maybe	Environment Agency (2003b)	These CAS nos. represent the commercial substance. BCF not fully reliable. Chronic toxicity estimated.

Table continued overleaf

Table 3.11 continued

Substance	CAS No.	Formula	Water Solubility	Log K_{ow}	Biodegradation	BCF	Lowest aquatic toxicity values (mg/l)		PBT?	Reference	Comment
							Acute	Chronic			
2,4,6-Tris(1,1-dimethylethyl) phenol	732-26-3	$C_{18}H_{30}O$	0.512 mg/l at 20°C	6.06	Not readily biodegradable (biodegrades in months[b])	23,200	0.061	0.003[a]	Maybe	ChemFinder; OSPAR Background document (2002)	Chronic toxicity estimated. OSPAR priority hazardous substance
2,4,6-Tri-*sec*-butylphenol	5892-47-7	$C_{18}H_{30}O$	0.21 mg/l[a]	6.5[a]	Biodegrades in weeks–months[b]	43,651[c]	0.065[a]	0.003[a]	Maybe		All data estimated
4-*sec*-Butyl-2,6-di-*tert*-butylphenol	17540-75-9	$C_{18}H_{30}O$	0.25 mg/l[a]	6.4[a]	Biodegrades in months[b]	42,072[c]	0.072[a]	0.003[a]	Maybe		All data estimated
Dinonylphenol	1323-65-5	$C_{24}H_{42}O$	See below (no data or estimate available)								Biodegradation, BCF and aquatic toxicity data estimated. BCF is unreliable. Could be persistent by analogy with nonylphenol
Phenol, 2,4-dinonyl branched	84852-14-2	$C_{24}H_{42}O$									
2,4-Dinonyl-phenol	137-99-5	$C_{24}H_{42}O$	2.8E-05 mg/l	10.5	Biodegrades in weeks[b]	99[c]	3×10^{-4}, [a]	3×10^{-5}, [a]	Maybe	WHO/IPCS/ILO International Chemical Safety Cards (2002); EPIWIN (2002)	

Table continued overleaf

Table 3.11 continued

Substance	CAS No.	Formula	Water Solubility	Log K_{ow}	Biodegradation	BCF	Lowest aquatic toxicity values (mg/l)		PBT?	Reference	Comment
							Acute	Chronic			
2,6-Di-*tert*-butyl-p-cresol	128-37-0	$C_{24}H_{42}O$	0.6 mg/l	5.1	Readily biodegradable (biodegrades in weeks–months[b])	2,500	1.4	0.316	No	IUCLID; ECOTOX; SRC PhysProp Database	Synonym: Butylated hydroxytoluene (BHT)
p-Hexyldecyl-phenol	2589-78-8	$C_{22}H_{38}O$	3.2×10^{-4} mg/l[a]	9.4[a]	Biodegrades in weeks[b]	2,311[c]	0.0012[a]	1.4×10^{-4} [a]	Maybe		Not commercially available, all data estimated. Could be persistent by analogy with dodecylphenol
2,6-Di-*tert*-butyl-4-nonylphenol	4306-88-1	$C_{23}H_{40}O$	6.7×10^{-4} mg/l[a]	8.96[a]	Biodegrades in weeks–months[b]	5,943[c]	0.003[a]	2.8×10^{-4}	Maybe		All data estimated
2,4,6-Tris(1-phenylethyl) phenol++	18254-13-2	$C_{30}H_{30}O$	8.6×10^{-3} mg/l	7.1[a]	Biodegrades in months[b]	44,874[c]	0.041[a]	0.002[a]	Maybe		All data estimated
Bis(*tert*-butyl)-dodecylphenol	68025-37-6	$C_{26}H_{46}O$	6.4×10^{-6} mg/l at 15°C	11.0[a]	Biodegrades in months[b]	16[c]	1.5×10^{-4} [a]	1.7×10^{-5} [a]	Maybe		All data estimated. BCF is unreliable.

Table continued overleaf

Table 3.11 continued

Substance	CAS No.	Formula	Water Solubility	Log K_{ow}	Biodegradation	BCF	Lowest aquatic toxicity values (mg/l)		PBT?	Reference	Comment
							Acute	Chronic			
Phenol, isopropylated	90480-88-9	$C_9H_{12}O$	~3% vol	2.97[a]	Biodegrades in weeks[b]	67[c]	2.9[a]	0.060[a]	No	IUCLID	Not commercially available now, all data estimated
Phenol, isobutylated	68610-06-0	$C_{10}H_{12}O$	330 mg/l[a]	3.45[a]	Biodegrades in weeks[b]	171[c]	2.0[a]	0.040[a]	No		All data estimated
Phenol, $C_{18–30}$ alkyl derivatives	68784-24-7	Unclear	No data or estimate available								Prediction difficult as structure is unclear
Phenol, styrenated ++	61788-44-1	Unclear	59 mg/l at 20°C	>4	Not readily biodegradable (biodegrades in weeks[b])	>501[c]	1–10	0.094[a]	Maybe	IUCLID	Chronic toxicity data estimated
Cumylphenol++	27576-86-9	$C_{15}H_{16}O$	See below								
4-Cumyl-phenol++	599-64-4	$C_{15}H_{16}O$	43 mg/l[a]	4.1[a]	Readily biodegradable (biodegrades in weeks–months[b])	610[c]	1.5[a]	0.029[a]	No	SDS; SASOL Report (modified Sturm test)	Water solubility, log K_{ow}, BCF and aquatic toxicity estimated

Table continued overleaf

Table 3.11 continued

Substance	CAS No.	Formula	Water Solubility	Log K_{ow}	Biodegradation	BCF	Lowest aquatic toxicity values (mg/l)		PBT?	Reference	Comment
							Acute	Chronic			
2-Cumyl-phenol++	18168-40-6	$C_{15}H_{16}O$	No data available								Properties expected to be similar to CAS 599-64-4 above
2,4-Di-cumene-phenol++	Unclear	$C_{20}H_{26}O$	No data or estimate available								

++ Aryl phenols rather than alkylphenols
SDS Safety data sheet produced by SASOL (SASOL, 2001)
[a] Values estimated using the Syracuse Research Corporation EPIWIN (V2.40) program
[b] Timeframe for ultimate biodegradation (mineralisation) estimated using the Syracuse Research Corporation BIOWIN (V3.63) program
[c] BCF values estimated from log K_{ow} using the methods outlined in the EU Technical Guidance Document

4 Analysis and discussion

4.1 General overview of the data

On the basis of data provided by industry only a limited number of alkylphenols are commercially important at the moment, and very few are produced or used at quantities greater than 1,000 tonnes/year in Europe. There may be significant variations in the cost of these substances due to the availability of feedstock. Only a few have appropriate physicochemical properties for consideration as substitutes for nonylphenol.

In general terms the amount of hazard data available (e.g. for biodegradation, bioaccumulation and toxicity) is very limited, although it is apparent that 4-alkylphenols become more toxic to aquatic organisms with increasing chain length. In addition, there is very little information about the environmental occurrence of most of these substances.

4.2 Hazard profiles for possible substitute alkylphenols

Eight alkylphenols were identified as possible substitutes for nonylphenol in Section 2. A number of factors were taken into account when selecting the substances: physicochemical properties, costs of feedstock, fitness of product, current commercial importance and scale of operation. 4-Cumylphenol has not been included here as this was outside the scope of this review (it is an arylphenol). For convenience, data for these substances are presented once more in this Section to provide more complete fate and hazard profiles than was possible in Table 3.11. These are shown in Table 4.1.

As described in Section 3.8, nonylphenol, 4-*tert*-octylphenol and dodecylphenol (branched) are similar in terms of the inherent hazard that they may present to the environment. All three are likely to partition similarly based on physicochemical properties and will also biodegrade slowly. They also have similar toxicity profiles (see Table 3.8). Dodecylphenol could be more bioaccumulative (although the measured BCF is not fully valid), and unlike the other two it meets the EU TGD screening criteria for consideration as a potential PBT substance.

Of the other candidates, the two mono-substituted butylphenols are readily biodegradable, and have higher water solubilities than all of the other substances (as would be expected with the shorter alkyl chain). In addition they are less hydrophobic, having lower log K_{ow} values, and consequently are less toxic (although endocrine disruption potential may need further assessment). They therefore appear to be of lesser environmental concern.

The remaining three substances are not readily biodegradable, and are therefore potentially persistent in the environment. They have moderate bioaccumulation potential (all except 2,4-di-*tert*-butylphenol which has a log K_{ow} value below 5, with measured or predicted BCFs around 500).[8] All three appear to be chronically toxic to aquatic organisms, with 'no effect concentrations' in the range of 60 μg/l or less. Their influence on the endocrine system is unclear. They are therefore potentially of similar concern to nonylphenol, and all are commercially important.

A more in-depth review of the data (with access to original study reports) would be prudent before firm conclusions are drawn for any of these potential substitutes.

[8] Two log K_{ow} values are given in Table 3.11 for 4-*tert*-pentylphenol – it is likely that the higher value (4.03) is more realistic, following the trend in the group (it is predicted to be 3.91 using the SRC EPIWIN suite).

Table 4.1 Hazard profiles for nonylphenol and potential substitute alkylphenols (est = estimated, meas = measured)

		2-*tert*-Butyl-phenol	**4-*tert*-Butyl-phenol**	**4-*tert*-Pentyl-phenol**	**4-*tert*-Octyl-phenol**	**Nonylphenol**	**Dodecyl-phenol (branched)**	**2,4-Di-*tert*-butyl-phenol**	**2,6-Di-*tert*-butyl-phenol**
Physicochemical properties									
Water solubility (mg/l)		700 (meas)	610 (meas)	37	19 (meas)	**6 (meas)**	1	12	4.11
Octanol-water partition coefficient (log K_{ow})		2.7–3.5	3.3	4.03	4.12	**4.48**	5.5	5.19	4.5
Persistence									
Biodegradation		Readily biodegradable	Readily biodegradable	Not readily biodegradable	Inherently biodegradable	**Inherently biodegradable**	Not readily biodegradable	Not readily biodegradable	Not readily biodegradable
Bioaccumulation									
Highest fish BCF value		188 (est)	120	531 (est)	634 (est)	**1,280**	9,440 (est)	~660 (est)	660
Toxicity									
Aquatic toxicity (mg/l)	Acute	2.4	3.4	1.7	0.013	**0.085**	0.093	1.8	0.076
	Chronic	0.042 (est)	0.73	0.063	0.006	**0.025**	No data available	0.008 (est)	0.019 (est)

5 Conclusions

The purpose of this review was to identify likely substitutes for nonylphenol in some or all of its uses, and to screen available data to prioritise candidates for further risk assessment activity. A large number of substances have been screened as part of this exercise, but it is important to note that the majority have very limited amounts of information available on their properties.

The major use of nonylphenol is in the manufacture of ethoxylate derivatives. Many of the applications of these derivatives will be banned in Europe in early 2005, and substitution activities are already under way (using long chain alcohols). Although other alkylphenol ethoxylates do exist commercially, they are unlikely to be important replacements, mainly due to economic factors (e.g. feedstock price) and handling differences. In the UK, the Chemicals Stakeholder Forum has reached a number of voluntary agreements with industry to avoid the replacement of nonylphenol with octylphenol in this application.

No suitable alternatives have so far been identified for phenolic oxime or tris(4-nonylphenyl)phosphite (TNPP) manufacture. The information presented by CEPAD suggests that only a limited number of alkylphenols are available as potential replacements for nonylphenol in some of its other applications. These are:

- 2-*tert*-butylphenol
- 4-*tert*-butylphenol (this is being assessed under the EU Existing Substances Regulation, so does not need further prioritisation)
- 4-*tert*-pentylphenol
- 4-*tert*-octylphenol
- dodecylphenol (branched)
- 2,4-di-*tert*-butylphenol
- 2,6-di-*tert*-butylphenol.

The two butylphenols are of lower environmental concern than nonylphenol, but the rest may pose similar hazards. They are all produced in quantities above 1,000 tonnes/year in Europe (with the exception of 4-*tert*-pentylphenol), and so have commercial markets already established. Even though the supply volume of 4-*tert*-pentylphenol is lower, it is still considered to be commercially important by CEPAD.

The substance that has the greatest potential to act as a substitute in general terms is 4-*tert*-octylphenol. However, its hazard profile is very similar to nonylphenol, so it is likely to pose the same level of risk in similar applications, at least at the local scale. Dodecylphenol might also be a substitute for more limited uses, although again its hazard profile is similar to nonylphenol.

2-*tert*-Butylphenol (CAS no. 88-18-6) has been assessed in Germany (BUA, 2001) and care must be taken to avoid duplication of effort with that report. There may also be potential for read-across from the ESR assessment of 4-*tert*-butylphenol in due course. Coupled with an environmental hazard profile that appears to be of less concern than nonylphenol, it is therefore of lower priority than the others for now.

Actual substitution will depend on a range of factors, including suitability of the final product for the intended use, and this report does not attempt to discuss this issue in any detail. Finally, it is not the intention of this report to imply that substitution will be straightforward or indeed possible in all cases.

6 Recommendations

1. Environmental risk assessment reports should be prepared for 4-*tert*-octylphenol (CAS no. 140-66-9) and dodecylphenol (branched) (CAS nos. 121158-58-5 & 74499-35-7) as a priority. This is because they are high volume substances with similar hazard profiles to nonylphenol, and they are also the most likely immediate replacements for nonylphenol. The evaluation should focus on the current use pattern for the substance, but in the case of 4-*tert*-octylphenol should also include a hypothetical use pattern that could arise if it were to replace nonylphenol in its current applications. **Note:** This work is already underway, because it was clear from the first draft of this report that assessments were needed. The draft reports are referenced in this report as Environment Agency, 2003a and 2003b. They will be published later in 2005.

2. Consideration should be given to alerting other regulatory authorities to the apparent PBT properties of dodecylphenol. If appropriate, industry should be invited to prepare an OECD hazard assessment for this substance under the ICCA HPV Challenge Programme (an OECD assessment already exists for 4-*tert*-octylphenol).

3. Risk assessments should also be undertaken for the remaining candidate nonylphenol substitutes, with priority given to the higher tonnage di-alkylphenols:

   - 4-*tert*-pentylphenol (CAS no. 80-46-6)
   - 2,4-di-*tert*-butylphenol (CAS no. 96-76-4)
   - 2,6-di-*tert*-butylphenol (CAS no. 128-39-2).

   The available data are insufficient to allow even a basic assessment for these substances at the moment, and this needs to be addressed first (e.g. by encouraging sponsorship through international hazard assessment initiatives,[9] or data call-in under the ESR).

   It might also be prudent to consider 4-*tert*-heptylphenol (CAS no. 1987-50-4) as part of a group assessment with 4-*tert*-pentylphenol, at least in terms of a hazard assessment, since it bridges the gap with octylphenol. Although it was considered to be commercially unimportant by CEPAD, the lubricant industry in the USA has submitted a test plan under the US HPV Chemical Challenge programme (which implies a major use in North America, which could be reflected in the EU). The full life cycle of any substance should be considered during the risk assessment stage.

4. 4-Cumylphenol (CAS no. 599-64-4) was identified by industry as having some potential to act as a substitute for nonylphenol in some uses.

[9] 2,4-Di-*tert*-butylphenol has been listed on the ICCA HPV Challenge website for some time, so it is likely that more data will become available in due course (although no sponsor has been identified).

Detailed consideration of this substance was outside the scope of this review, but consideration could be given to obtaining more information on this substance and reviewing its hazard profile (it does not appear to be a PBT candidate substance).

5. Finally, a number of other substances that were considered during the initial data screening have been highlighted as potential PBT substances yet do not appear to have any risk assessment available. Pending a more detailed analysis of the data, consideration could be given to alerting other regulatory authorities to their PBT properties. The substances are:

   - 2,4-Di-*tert*-pentylphenol (CAS no. 120-95-6)
   - 2,6-Di-*tert*-butyl-4-ethy phenol (CAS no. 4130-42-1)
   - 2,4,6-Tri-*sec*-butylphenol (CAS no. 5892-47-7)
   - 4-*sec*-Butyl-2,6-di-*tert*-butylphenol (CAS no. 17540-75-9)
   - 2,4-Dinonylphenol (branched) (CAS no. 84852-14-2, also 137-99-5 & 1323-65-5)
   - 4-Hexyldecylphenol (CAS no. 2589-78-8)
   - 2,6-Di-*tert*-butyl-4-nonyl phenol (CAS no. 4306-88-1)
   - 2,4,6-Tris(1-phenylethyl) phenol (CAS no. 18254-13-2)
   - Bis(*tert*-butyl)-dodecylphenol (CAS no. 68025-37-6)
   - Phenol, styrenated (CAS no. 61788-44-1).

   Based on data from CEPAD, only 2,4-di-*tert*-pentylphenol, dinonylphenol and styrenated phenol are considered to have commercial importance – an environmental risk assessment might be useful for these. However, they are also believed to be fairly low tonnage substances, and so they are not the highest priority for assessment compared with the other substances identified in this section.

References

Blackburn, M. A. and Waldock, M. J. (1995) Concentrations of alkylphenols in rivers and estuaries in England and Wales. *Water Research*, **29**, 1623–1629.

BUA (2001) 2-tert-Butylphenol. BUA Stoffbericht 231. February 2001.

Buffagni, M., Cova, C. A., Bracco, L. and Giacca, D. (2001) Acute ecotoxicological effects of alkylated phenols in produced water discharged at sea-model inputs to DREAM project. Poster, 11th SETAC Europe Annual Meeting, Congress Hall, Madrid, Spain, 6–10 May 2001.

CERI (2001) Development of competitive binding assay to the medaka (*Oryzias latipes*) estrogen receptor α. Chemicals Evaluation and Research Institute, Japan.

CHEMFINDER http://chemfinder.cambridgesoft.com/

Danish Ministry of the Environment (1997) Submission of monitoring data to the COMPPS database.

Department of Environment, Transport and the Regions (DETR) (1999) Nonylphenol Risk Reduction Strategy, prepared by Risk and Policy Analysts.

ECB (1999) European Union Risk Assessment Report: 4-nonylphenol (branched) and nonylphenol. Draft, September 1999. European Chemicals Bureau, 2nd Priority List. Available from: http://ecb.ei.jrc.it/existing-chemicals/.

Environment Agency (1999) Endocrine-disrupting substances in the environment: The Environment Agency's strategy. Environment Agency, Bristol.

Environment Agency (2003a) Risk Assessment Report: 4-*tert*-octylphenol. Unpublished draft, July 2003.

Environment Agency (2003b) Risk Assessment Report: dodecylphenol, mixed isomers (branched). Unpublished draft, August 2003.

EPIWIN – Syracuse Research Corporation program http://www.epa.gov/oppt/p2framework/docs/epiwin.htm.

Gerritsen, A., van der Hoeven, N. and Pielaat, A. (1998) The acute toxicity of selected alkylphenols to young and adult *Daphnia magna*. *Ecotoxicology and Environmental Safety*, **39**(3), 227–232.

Gimeno, S., Gerritsen, A., Bowmer, T. and Komen, H. (1996) Feminization of male carp. *Nature*, **384**, 221–222.

HSDB (2002) http://www.nlm.nih.gov/pubs/factsheets/hsdbfs.html

IRPTC Data profile http://www.chem.unep.ch/irptc/

IUCLID (2000) International Uniform Chemical Information Database, CD ROM 2000 Edition (some data also from confidential version of database).

KEMI (2000) Risk Assessment of Alkylphenol and Alkylphenol Ethoxylate Exposure, With Focus on Octylphenol and Butylphenol. OSPAR Convention for the Protection of the Marine Environment of the North-East Atlantic. Programmes and Measures Committee (PRAM) 10–14 April 2000. PRAM 00/3/Info.2-E (L).

McLeese, D. W., Zitko, V., Sergeant, D. B., Burridge, L. and Metcalfe, C. D. (1981) Lethality and accumulation of alkylphenols in aquatic fauna. *Chemosphere*, **10**, 723–730.

NCEDS (1999) Monitoring Data for Octylphenol in Trade Effluent, Sewage Effluent and Surface Waters on the Wyre Peninsula. UK Environment Agency National Centre for Environmental Data and Surveillance.

NTP: http://ntp-server.niehs.nih.gov/

OSPAR (2000) Briefing document on the work of Dynamec and the Dynamec Mechanism for the Selection and Prioritisation of Hazardous Substances.

SASOL (2001) EC Safety Data Sheets for Alkylphenols. Revised August 2001.

SEPA (1997) Environmental concentrations of endocrine disrupting chemicals at selected sites in Scotland. SEPA Internal Report.

SIDS and SIARs (various dates) Screening Information Data Sheets and SIDS Initial Assessment Reports, various substances, OECD HPV programme.

SRC PhysProp Database http://www.syrres.com/esc/physdemo.htm

TGD (2003) Technical Guidance Document (Second Edition), Parts I-IV, EUR 20418 EN/1-4

UBA (1999) Organisches Zinnverbindungen, Alkylphenole und Bisphenol-A in marinen und limnishen Biota der Umweltprobenbank. Methodische Entwicklungen sowie aktuelles und retrospectives Monitoring. Forschungsbericht 297 63 155, UBA-FB 000020.

USEPA (2001) Robust Summary and Test Plan Data submitted by Schenectady International under the HPV Challenge Program. AR 201-13007, April 2001. http://www.hpvchallenge.com/

Waern, F. (2000) Risk Assessment of Alkylphenol and Alkylphenol Ethoxylate Exposure, with focus on Octylphenol and Butylphenol. Institute of Environmental Medicine, Karolinska Institutet, Stockholm, Sweden

WHO/IPCS/ILO: http://www.inchem.org/

Working Group for the Cleanliness of the Elbe (1998) Endocrine effects substances in the Elbe, its tributaries, and in the North Sea.

Yoshioka, Y., Ose, Y. and Sato, T. (1985) Testing for the toxicity of chemicals with *Tetrahymena pyriformis*. *Science of the Total Environment*, **43**, 149–157.

Annex I Alkylphenol datasheets

Note of caution: The following data sheets have been prepared following a review of data from a variety of sources during 2002. In many cases it has not been possible to review the original data source, nor comment on the likely test substance composition. The sheets do not represent in-depth reviews of the data (for example as might be required for a risk assessment), and should therefore be used as a guide only. The data sheet for 4-*tert*-butylphenol does not take account of the EU draft risk assessment that has recently been circulated for comment under the Existing Substances Regulation.

A number of symbols have been used to save space. An explanation is given below:

1 = Carried out to standard guidelines
2 = Deemed to be appropriate/good quality (although not to a standard guideline)
3 = Limited or poor quality study
4 = Full study not obtained

UP = unpublished
IS = insufficient data to assess
Cal = Calculated

Data sheets are not presented for 4-*tert*-octylphenol or dodecylphenol (branched), since these substances are already subject to a detailed risk assessment by the Environment Agency (2003a and 2003b), as a consequence of an earlier draft of this report. The detailed data review in those assessments supersedes the preliminary information provided by the data sheets in this annex.

Substance: **4-*tert*-Butylphenol** **CAS No.: 98-54-4**
Formula: **$C_{10}H_{14}O$** **Molecular weight: 150.2**

Data type	Protocol	Results	Ref	Quality
Physical-chemical				
Melting point	Not known	99.3°C	c	4/IS
		c. 100°C	d,e	4/IS
Boiling point	Not known	237°C at 1013 hPa	b,c	4/IS
Density	Not known	0.92 g/m^3 at 110°C	c	4/IS
Vapour pressure	Not known	1.3x10^2 Pa at 70°C	c	4/IS
		0.5 Pa at 20°C	d	4/IS
Water solubility	OECD TG 105	610 mg/l at 25°C	c	1/4
	Other	800 mg/l at 20°C	d	4/IS
	Other	500 mg/l	e	4/IS
Partition coefficient (log K_{ow})	OECD TG 107	3.29 at 25°C	c	1
	Other (shake flask)	3.31	d	4/IS
Environmental fate and pathway				
Photodegradation	AOPWIN v 1.88 indirect photolysis, OH radicals	Half-life = 3.16 hours	d	4/IS/Cal
Stability in water	OECD TG 111	Stable at pH 4, 7 & 9	c	1/4
Transport and distribution	Fugacity, Mackay Level III type Release: 100% to water	Air: 18.9% Water: 79.1% Sediment: 1.3% Soil: 0.7%	c	Cal
Biodegradation	OECD TG 301C	Not readily biodegradable	c	1/4
	OECD TG 301A	Readily biodegradable, >70% in 28 days	e	1/4
Bioaccumulation	Other (Static test)	BCF = 120	b,c	4/IS
Ecotoxicology				
Toxicity to fish	OECD TG 203	96-h LC50 = 5.1 mg/l *Oryzias latipes*	c	1/4
Toxicity to aquatic invertebrates	OECD TG 202	48-h EC50 = 3.4–3.9 (*Daphnia magna* immobilisation)	b,c	1/4

Data type	Protocol	Results	Ref	Quality
		21-d NOEC = 0.73 mg/l (*Daphnia magna* repro.)		
Toxicity to aquatic plants	OECD TG 201	72-h EC50 = 11.0 mg/l *Scenedesmus subspicatus*	b,c	1/4
		72-h NOEC = 9.53 mg/l (growth inhibition) *Selenastrum capricornutum*		
Mammalian toxicology				
Acute oral toxicity	OECD TG 401	Rat LD50 = 4,000 mg/kg bw	b	1/4
Oestrogenic activity	E Screen (potency of oestradiol = 100)	Relative potency = 0.0003	b	4/IS
	Yeast screen	Relative potency = 0.2		

References:

(a) IUCLID; (b) Waern (2000); (c) SIDS; (d) US EPA (2001); (e) SASOL (2001)

SUBSTANCE: 2-*tert*-Butylphenol **CAS NO: 88-18-6**
FORMULA: $C_{10}H_{14}O$ **Molecular weight: 150.22**

Data type	Protocol	Results	Ref	Quality
Physical-chemical				
Melting point	Not known	-7 to -6.8°C	a, b	4/IS
Boiling point	Not known	221 to 223°C	a, b	4/IS
Density	Not known	0.978 g/cm^3	a	4/IS
Vapour pressure	Not known	0.09 mmHg (0.12 hPa) at 25°C	e	4/IS
		0.05 hPa at 20°C	f	4/IS
Water solubility	Other (experimental)	700 mg/l at 25°C	b	4/IS
		394 mg/l at 25°C	e	4/IS
		2,300 mg/l at 20°C	f	4/IS
Partition coefficient (log K_{ow})	Other (experimental)	3.31	b, f	4/IS
		3.43 to 3.52	d	4/IS
Environmental fate and pathway				
Photodegradation	AOPWIN v 1.88 indirect photolysis, OH radicals	Half-life = 3.16 hours	f	4/IS/Cal
Stability in water	No data	No data		
Transport and distribution	Fugacity, Mackay Level I type	Air: 27% Water: 26% Sediment: 1% Soil: 46%	e	4/IS/Cal
Biodegradation	OECD TG 301A	Readily biodegradable, >70% in 28 days	f	1/4
Bioaccumulation	TGD QSAR (quantitative structure–activity relationship)	BCF = 39–188	g	2/Cal
Ecotoxicology				
Toxicity to fish	Not known	48-h LC50 = 3.7 mg/l *Leuciscus idus*	d	4/IS
	Other (predicted)	60 d NOEC = 0.042 mg/l	g	2/Cal
Toxicity to aquatic invertebrates	Not known	48-h EC50 = 3.4 mg/l *Daphnia magna*	d	4/IS

Data type	Protocol	Results	Ref	Quality
	Other (Static)	96-h LC50 = 2.4 mg/l *Crangon septemspinosa*	c	3
Toxicity to aquatic plants	Not known	72-h EC50 = 3.1 mg/l *Scenedesmus subspicatus*	d	4/IS
Mammalian toxicology				
Acute oral toxicity	OECD 401	Rat LD50 = 200–2,000 mg/kg bw	f	1/4
		Rat LD50 = 789 mg/kg bw	e	1/4
Oestrogenic activity	No data	No data		

References:
(a) ChemFinder; (b) SRC PhysProp Database; (c) McLeese *et al.* (1981); (d) BUA (2001); (e) USEPA (2001); (f) SASOL (2001); (g) this report

SUBSTANCE: **2-*sec*-Butylphenol** **CAS No.: 89-72-5**
FORMULA: **$C_{10}H_{14}O$** **Molecular weight: 150.22**

Data type	Protocol	Results	Ref	Quality
Physical-chemical				
Melting point	Not known	12 to 16°C	a, b	4/IS
		14°C	e	4/IS
Boiling point	Not known	227–228°C	a, b	4/IS
		224°C	e	4/IS
Density	Not known	0.98 g/cm^3	a	4/IS
Vapour pressure	Other (estimated)	0.05 mmHg (6.7 Pa) at 25°C	b	4/IS
		0.0173 mmHg (2.31 Pa) at 25°C	e	4/IS
Water solubility	Other (estimated)	1,659 mg/l at 25°C	b	4/IS
		319 mg/l at 25°C	e	4/IS
Partition coefficient (log K_{ow})	Other (experimental)	2.8	d	3
		3.27	b	4/IS
		3.46	e	4/IS
Environmental fate and pathway				
Photodegradation	AOPWIN v 1.88 indirect photolysis, OH radicals	Half-life = 2.9 hours	e	4/IS/Cal
Stability in water	No data	No data		
Transport and distribution	Fugacity, Mackay Level I type	Air: 7.5% Water: 34% Sediment: 1.5% Soil: 57%	e	4/IS/Cal
Biodegradation	Other (predicted)	Biodegrades in weeks	f	2/Cal
Bioaccumulation	TGD QSAR	48–174	f	2/Cal
Ecotoxicology				
Toxicity to fish	Other (predicted)	60-d NOEC = 0.040 mg/l	f	2/Cal
Toxicity to aquatic invertebrates	Other (Static)	96-h LC50 = 1.3 mg/l *Crangon septemspinosa*	d	3
Toxicity to aquatic plants	No data	No data		

Data type	Protocol	Results	Ref	Quality
Mammalian toxicology				
Acute oral toxicity	Not known	Rat LD50 = 2,700 mg/kg bw	c	4/IS
		Rat LD50 = 200-2,000 mg/kg bw	e	1/4
Oestrogenic activity	No data	No data		

References:
(a) ChemFinder; (b) SRC PhysProp Database; (c) NTP Chemical Repository; (d) McLeese *et al.* (1981); (e) USEPA (2001); (f) this report

SUBSTANCE: **4-*tert*-Pentylphenol** **CAS No.: 80-46-6**
FORMULA: **$C_{11}H_{16}O$** **Molecular weight: 164.25**

Data type	Protocol	Results	Ref	Quality
Physical-chemical				
Melting point	Not known	91 to 94°C	a	4/IS
		94 to 95°C	f	4/IS
Boiling point	Not known	255°C	a	4/IS
		256°C	f	4/IS
		262.5°C	e	4/IS
Density	Not known	0.9624 g/cm^3 at 20°C	b	4/IS
		0.922 g/cm^3 at 100°C	f	4/IS
Vapour pressure	Other	0.00783 mmHg (1.04 Pa) at 25°C	e	4/IS
		3.1 hPa at 100°C	f	4/IS
Water solubility	Not known	168 mg/l at 25°C	e	4/IS
		37 mg/l at 20°C	f	4/IS
Partition coefficient (log K_{ow})	Not known	2.1	c	3
		4.03	e	4/IS
Environmental fate and pathway				
Photodegradation	AOPWIN v 1.77 indirect photolysis, OH radicals	Half-life = 3.07 hours	e	4/IS/Cal
Stability in water	No data	No data		
Transport and distribution	Fugacity, Mackay Level III type Release: 100% to water	Air: 2% Water: 9% Sediment: 2% Soil: 87%	e	4/IS
Biodegradation	OECD TG 301B	Not readily biodegradable, <70% in 28 days	f	1/4
Bioaccumulation	TGD QSAR	BCF = 531	g	2/Cal
Ecotoxicology				
Toxicity to fish	Other (unknown)	96-h LC50 = 1–10 mg/l *Cyprinus carpio*	f	4/IS
	Other	30-d EC50 (oviduct formation in male fish) = 63 μg/l	d	2

Data type	Protocol	Results	Ref	Quality
Toxicity to aquatic invertebrates	Other (not known)	48-h EC50 = 1–10 mg/l *Daphnia magna*	f	4/IS
	Other (static)	96-h LC50 = 1.7 mg/l *Crangon septemspinosa*	c	3
Toxicity to aquatic plants	Other (not known)	72-h EC50 = 1–10 mg/l *Scenedesmus subspicata*	f	4/IS
Mammalian toxicology				
Acute oral toxicity	Not known	Rat LD50 = 1,830 mg/kg bw	b	4/IS
Oestrogenic activity	No data	No data, but see fish result		

References:
(a) ChemFinder; (b) NTP; (c) McLeese *et al.* (1981); (d) Gimeno *et al.* (1996); (e) USEPA (2001); (f) SASOL (2001); (g) this report

SUBSTANCE: **2-*tert*-Butyl-4-methylphenol** **CAS No.: 2409-55-4**
FORMULA: **$C_{11}H_{16}O$** **Molecular weight: 164.27**

Data type	Protocol	Results	Ref	Quality
Physical-chemical				
Melting point	Not known	49–52°C	a	4/UP
Boiling point	Not known	237°C	a	4/UP
Density	Not known	0.924 g/cm^3 at 20°C	a	4/UP
Vapour pressure	Not known	75 hPa at 75°C	a	4/UP
Water solubility	Other (predicted)	101 mg/l at 25°C	b	2/Cal
Partition coefficient (log K_{ow})	Other (predicted)	4.0	b	2/Cal
Environmental fate and pathway				
Biodegradation	Other (predicted)	Biodegrades in weeks–months	b	2/Cal
Ecotoxicology				
Toxicity to fish	Other (predicted)	60-d NOEC = 0.026 mg/l	b	2/Cal
Toxicity to aquatic invertebrates	Other (predicted)	48-h LC50 = 1.4 mg/l *Daphnia magna*	b	2/Cal
Mammalian toxicology				
Acute oral toxicity	Not known	Rat LD50 = 2,390–2,500 mg/kg bw	a	4/IS
Oestrogenic activity	No data	No data		

References:
(a) IUCLID (non-confidential); (b) this report

SUBSTANCE: 2,6-Di-*tert*-butylphenol **CAS No.: 128-39-2**
FORMULA: $C_{14}H_{22}O$ **Molecular weight: 206.33**

Data type	Protocol	Results	Ref	Quality
Physical-chemical				
Melting point	Not known	36 to 37°C	c, e	4/IS
Boiling point	Not known	253°C at 101.3 kPa	c, e	4/IS
Vapour pressure	Other (gas saturation method)	0.0076 mmHg (1.01 Pa) at 20°C	c, e	4/UP
Water solubility	Generator Column Method	4.11 mg/l at 25°C & pH 7	c, e	4/IS
Partition coefficient (log K_{ow})	OECD TG 117	4.5	c	1/4/UP
Environmental fate and pathway				
Photodegradation	AOPWIN v 1.88 indirect photolysis, OH radicals	Half-life = 2.4 hours	e	4/IS/Cal
	EPA TSCA 40 CFR 795-70	Half life = 2.6 hours for a 12 hour day (5.2 hours for a 24 hour day)	d, e	4/Cal
Stability in water	Not known	Unstable (no further data available)	b	4/UP/IS
Transport and distribution	Fugacity, Mackay Level I type	Air: 26% Water: 2% Sediment: 2% Soil: 70%	d, e	4/Cal
Biodegradation	OECD TG 301 B (modified Sturm Test)	4% and 1% biodegradation after 28 days at 10 and 20 mg/l, respectively	c, e	1/4/UP
	TSCA 796.3140	0% biodegradation after 56 days	e	1/4
Bioaccumulation	Measured	Golden orfe BCF = 660 (after 3 days)	c	4/IS
Ecotoxicology				
Toxicity to fish	OECD 203 (static)	96-h LC50 =13 mg/l *Brachydanio rerio*	c	1/4/UP
	Annex V, C1 (static)	96-h LC50 = 7.6 mg/l	e	1/4/UP
	Other (predicted)	60-d NOEC = 0.019 mg/l	f	2/Cal

Data type	Protocol	Results	Ref	Quality
Toxicity to aquatic invertebrates	OECD TG 202	24-h EC50 = 1.7 mg/l *Daphnia magna*	c, e	1/4/UP
	US standards	48-h NOEC= 0.076 mg/l	c	1/4/UP
Toxicity to aquatic plants	EPA TSCA 797.1050 (static)	96-h EC50 = 0.56 mg/l *Selenastrun capricornutum*	e	1/4/UP
Mammalian toxicology				
Acute oral toxicity	Other	Rat LD50 > 5,000 mg/kg bw	c	4/UP/IS
Oestrogenic activity	No data	No data		

References:
(a) IUCLID confidential; (b) IRPTC Data profile; (c) SIDS; (d) Revised SIAR;
(e) USEPA (2001); (f) this report

SUBSTANCE: 2,4-Di-*tert*-butylphenol **CAS No.: 96-76-4**
FORMULA: $C_{14}H_{22}O$ **Molecular weight: 206.33**

Data type	Protocol	Results	Ref	Quality
Physical-chemical				
Melting point	Not known	52 to 57°C	a, b	4/UP
Boiling point	Not known	265°C	a, c	4/UP
		264°C	c, d	4/IS
Density	Not known	0.935 g/cm^3 at 20°C	b	4/UP
Vapour pressure	Not known	1.0 Pa at 20°C	b	4/IS
Water solubility	Not known	12 mg/l at 20°C	b	4/UP
Partition coefficient (log K_{ow})	Other (calculated)	5.13	c	4/UP
		5.33	c	4/IS
Environmental fate and pathway				
Photodegradation	AOPWIN v 1.88 indirect photolysis, OH radicals	Half-life = 2.61 hours	c	4/IS/Cal
	Other (calculated)	Half-life = 0.3 days	b	4/UP/Cal
Stability in water	No data	No data		
Transport and distribution	Fugacity, Mackay Level I type	Air: 21.8% Water: 3.6% Sediment: 36% Soil: 35.5% Biota:2.4%	b	4/UP
Biodegradation	ISO Draft 'BOD test for insoluble substances 1990'	2% after 28 days (aerobic, activated sludge)	b	1/UP/4
Bioaccumulation	TGD QSAR	BCF = 5,146	e	2/Cal
Ecotoxicology				
Toxicity to fish	Other (Static, DIN38412 part 15)	48-h LC50 = 1.8 mg/l *Leuciscus idus*	b	1/UP/4
	Other (predicted)	60-d NOEC = 0.008 mg/l	e	2/Cal
Mammalian toxicology				
Acute oral toxicity	OECD TG 401	Rat LD50 = 2,559–4,128 mg/kg bw	b	1/UP/4
	EPA CFR 163.81-1	Rat LD50 = 1,500 mg/kg bw	c	1/4/UP

Data type	Protocol	Results	Ref	Quality
Oestrogenic activity	No data	No data		

References:
(a) ChemFinder; (b) IUCLID (non-confidential); (c) USEPA (2001); (d) SASOL (2001); (e) this report

Substance: **2,4-Di-*tert*-pentylphenol** **CAS No.: 120-95-6**
Formula: **$C_{16}H_{26}O$** **Molecular weight: 234.38**

Data type	Protocol	Results	Ref	Quality
Physical-chemical				
Melting point	Not known	26°C	a, b	4/IS
Boiling point	Not known	311°C	b	4/IS
Density	Not known	0.91 g/cm^3 at 50°C	a	4/IS
Vapour pressure	Not known	<0.01 hPa at 20°C	a	4/IS
		0.011 Pa at 25°C	b	4/IS
Water solubility	Not known	15 mg/l at 20°C	a	4/IS
		0.44 mg/l at 25°C	b	4/IS
Partition coefficient (log K_{ow})	Calculated	6.31	b	4/IS/Cal
Environmental fate and pathway				
Photodegradation	AOPWIN v 1.88 indirect photolysis, OH radicals	Half-life = 2.5 hours	b	4/IS
Stability in water	No data	No data		
Transport and distribution	Fugacity, Mackay Level I type Release: 100% to water	Air: 0.1% Water: 0.1% Sediment: 2.2% Soil: 97.6%	b	4/IS
Biodegradation	Not known	Not readily biodegradable	a	4/IS
Bioaccumulation	TGD QSAR	BCF = 40,381	c	2/Cal
Ecotoxicology				
Toxicity to fish	Other (predicted)	60-d NOEC = 0.003 mg/l	c	2/Cal
Toxicity to aquatic invertebrates	OECD TG 202	48-h EC50 = 1–10 mg/l *Daphnia magna*	a	4/IS
Mammalian toxicology				
Acute oral toxicity	OECD TG 401	Rat LD50 = 200–2,000 mg/l	a	4/IS
Oestrogenic activity	No data	No data		

References:
(a) SASOL (2001); (b) USEPA (2001); (c) this report

SUBSTANCE: 2,4-Dinonylphenol **CAS No.: 137-99-5**
FORMULA: $C_{24}H_{42}O$ **Molecular weight: 346.59**

Data type	Protocol	Results	Ref	Quality
Physical-chemical				
Melting point	Other (estimated)	162.6°C	b	Cal
Boiling point	Not known	430°C	b	Cal
Vapour pressure	Not known	1.1e-08 mmHg	b	Cal
Water solubility	Other (calculated)	2.8E-05 mg/l	b	Cal
Partition coefficient (log K_{ow})	Other (calculated)	10.5	b	Cal
Environmental fate and pathway				
Photodegradation	AOPWIN v 1.88 indirect photolysis, OH radicals	Half-life = 1.8 hours	b	Cal
Stability in water	No data	No data		
Biodegradation	Other (predicted)	Biodegrades in weeks	c	2/Cal
Bioaccumulation	TGD QSAR	BCF = 99	c	2/Cal
Ecotoxicology				
Toxicity to fish	Other (predicted	96-h LC50 = 3×10^{-4} mg/l	c	2/Cal
Toxicity to aquatic invertebrates	Other (predicted)	21-d NOEC = 3×10^{-5} mg/l	c	2/Cal
Mammalian toxicology				
No data				

References:
(a) HSDB (2002); (b) EPIWIN; (c) this report

SUBSTANCE: Styrenated phenol **CAS No.: 61788-44-1**
FORMULA: Complex **Molecular weight: Complex**

Data type	Protocol	Results	Ref	Quality
Physical-chemical				
Melting point	No data	No data		
Boiling point	Not known	200–250°C	a	UP
Density	Other	1.08 g/cm^3	a	4/UP
Vapour pressure	No data	No data		
Water solubility	Not known	59 mg/l at 20°C	a	4/UP
Partition coefficient (log K_{ow})	Other (experimental)	> 4 at 22°C	a	4/UP
Environmental fate and pathway				
Biodegradation	OECD TG 301	Biodegradation 7% after 28 days	a	4/UP
Bioaccumulation	Other (predicted)	BCF >501	b	2/Cal
Ecotoxicology				
Toxicity to fish	Other (static)	96-h LC50 = 1–10 mg/l *Brachydanio rerio*	a	4/UP
	Other (predicted)	60 d NOEC = 0.094 mg/l	b	2/Cal
Mammalian toxicology				
Acute oral toxicity	Not known	Rat LD50 = 2,500 mg/kg bw	a	4/UP
Oestrogenic activity	No data	No data		

References:
(a) IUCLID non-confidential; (b) this report

SUBSTANCE: Isopropylated phenol **CAS No.: 90480-88-9**
FORMULA: Mixture **Molecular weight: Mixture**

Data type	Protocol	Results	Ref	Quality
Physical-chemical				
Melting point	No data	No data		
Boiling point	Not known	>180°C	a	4/IS
Density	Not known	1 g/cm^3	a	4/IS
Vapour pressure	No data	No data		
Water solubility	Not known	Approximately 3% vol	a	4/IS
Partition coefficient (log K_{ow})	Other (predicted)	2.9	b	2/Cal
Environmental fate and pathway				
Biodegradation	Other (predicted)	Biodegrades in weeks	b	2/Cal
Bioaccumulation	TGD QSAR	BCF = 67	b	2/Cal
Ecotoxicology				
Toxicity to fish	Other (predicted)	60-d NOEC = 0.060 mg/l	b	2/Cal
Toxicity to aquatic invertebrates	Other (predicted)	48-h EC50 = 2.9 mg/l *Daphnia magna*	b	2/Cal
Mammalian toxicology				
No data				

References:
(a) IUCLID non-confidential; (b) this report

SUBSTANCE: 2,6-Di-*tert*-butyl-4-methylphenol (BHT) CAS No.: 128-37-0
FORMULA: $C_{15}H_{24}O$ Molecular weight: 220.35

Data type	Protocol	Results	Ref	Quality
Physical-chemical				
Melting point	Not known	70°C	a	4/UP
Boiling point	Not known	265°C	a	4/UP
Density	Not known	1.03 g/cm^3 at 20°C	a	4/UP
Vapour pressure	Not known	0.013 hPa at 20°C	a	4/UP
Water solubility	Not known	0.6 mg/l at 25°C	a	4/UP
Partition coefficient (log K_{ow})	Other	4.17 to 5.1 (measured)	a	4/UP
		5.6–6.2 (calculated)		
Environmental fate and pathway				
Photodegradation	Not known	Exposure to light said to accelerate degradation (no further data available)	a	4/UP/IS
Stability in water	Not known	Unstable (no further data available)	a	4/UP/IS
Biodegradation	OECD TG 301 D	<10% after 20 days (predominantly domestic sewage)	a	1/4/UP
Bioaccumulation	Guideline corresponding to OECD TG 305C	*Cyprinus carpio* BCF = 230–2,500 (56-d exposure to 50 μg/l)	a	1/4/IS
Ecotoxicology				
Toxicity to fish	OECD TG 204	14-d LC10 interpreted as 5 mg/l *Oncorhynchus mykiss*	a	1/4/UP
Toxicity to aquatic invertebrates	OECD TG 202	21-d LOEC = 1 mg/l (*Daphnia magna* reproduction)	a	1/4/UP
Mammalian toxicology				
Acute oral toxicity	Other	Rat LD50 = 890 to >10,000 mg/kg bw	a	4/IS
Oestrogenic activity	No data	No data		

References:
(a) IUCLID non-confidential; (b) Yoshioka *et al.* (1985)

Glossary of terms

Term	Description
Biochemical oxygen demand (BOD)	A measure of degradation potential
Bioconcentration factor (BCF)	A measure of chemical uptake, being 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
Lowest observed effect concentration	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, etc., as measured by laboratory screening tests involving micro-organisms

List of abbreviations

Acronym	Description
AP	Alkylphenol
ASTM	American Society for Testing and Materials
BCF	Bioconcentration factor
BHT	Butylated hydroxytoluene; systematic name 2,6-di-*tert*-butyl-p-cresol; CAS no. 128-37-0
BOD	Biochemical oxygen demand
BUA	Beratergremium für Altstoffe – the Advisory Committee on Existing Chemicals of the Association of German Chemists (GDCh)
bw	Body weight
CAS	Chemical Abstract Services
CEPAD	Conseil Européen des Phénols Alkylés et Derivés (the European Council for Alkylphenols and Derivatives): a trade association representing the major European producers of alkylphenols, and some of the users (http://www.cefic.be/cepad/)
DIN	Deutsche Industrie Norm (German norm)
ECB	European Chemicals Bureau
EC	European Communities
EC_{50}	Median effective concentration
EC_x	As EC_{50}, but for x% effect; x usually being 0, 10, or 100
EEC	European Economic Communities
EPA	Environmental Protection Agency (USA)
EQS	Environmental quality standard
ESR	Existing Substances Regulation (ESR): Council Regulation (EEC) 793/93 on the evaluation and control of the risks of existing substances
EU	European Union
HPV	High production volume (> 1,000 tonnes/year)
HSDB	Hazardous Substances Data Bank
ILO	International Labour Organisation
IPC	Integrated Pollution Control
IPCS	International Programme on Chemical Safety
IPPC	Industrial Pollution Prevention and Control (EC Directive 96/61/EEC)
IRPTC	International Register of Potentially Toxic Chemicals
ISO	International Organisation for Standardisation
IUCLID	International Uniform Chemical Information Database: contains data collected under the Existing Substances Regulation (ESR)

Acronym	Description
LC_{50}	Median lethal concentration
LD_{50}	Median lethal dose
LOEC	Lowest observed effect concentration
log K_{ow}	Log of the octanol-water partition coefficient (K_{ow})
MW	Molecular weight
NCEDS	National Centre for Environmental Data and Surveillance, Environment Agency (this has since become part of the Science Group)
NOEC	No observed effect concentration
NP	Nonylphenol
NTP	National Toxicology Program (USA)
OECD	Organisation for Economic Co-operation and Development
OP	4-*tert*-Octylphenol
OSPAR	Oslo and Paris Convention for the Protection of the Marine Environment of the Northeast Atlantic
PBT	Persistent, bioaccumulative and toxic
pH	Logarithm (to the base 10) (of the hydrogen ion concentration {H+}
(Q)SAR	(Quantitative) structure–activity relationship
RBA	Relative binding affinity
SDS	Safety data sheet
SEPA	Scottish Environment Protection Agency
SETAC	Society for Environmental Toxicology and Chemistry
SIDS	Screening Initial Data Set (a basic hazard assessment)
STW	Sewage treatment works
TG	Test guideline
TGD	Technical guidance document
UBA	Umwelt Bundesamt – the German Federal Environmental Agency
US EPA	Environmental Protection Agency, USA
UV	Ultraviolet region of the electromagnetic spectrum
vPvB	Very persistent and very bioaccumulative
WHO	World Health Organization

We welcome views from our users, stakeholders and the public, including comments about the content and presentation of this report. If you are happy with our service, please tell us about it. It helps us to identify good practice and rewards our staff. If you are unhappy with our service, please let us know how we can improve it.