SCREENING-LEVEL HAZARD CHARACTERIZATION AND PRIORITIZATION

ALKYL PHENOLS
8 Chemicals

HBP Subject Chemicals

CAS Registry Number	CA[1] Index Name
91672-41-2	Phenol, 2-nonyl-, branched
134701-20-5	Phenol, 2,4-dimethyl-6-(1-methylpentadecyl)-
233587-36-5	Phenol, 2(or 4)-sec-tetracosyl-
234446-37-8	Phenol, 2(or 4)-sec-hexacosyl-
234446-38-9	Phenol, 2(or 4)-sec-octacosyl-
234446-39-0	Phenol, 2(or 4)-sec-triacontyl-

Supporting Chemicals

CAS Registry Number	CA[1] Index Name
89-72-5	Phenol, 2-(1-methylpropyl)-
84852-15-3	Phenol, 4-nonyl-, branched

Prepared by
Office of Pollution Prevention and Toxics
Environmental Protection Agency
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[1] Chemical Abstracts

SCREENING-LEVEL HAZARD CHARACTERIZATION AND PRIORITIZATION DOCUMENT

Screening-level hazard characterizations for medium production volume chemicals are important contributions to the chemicals cooperation work being done in North America[2] through the EPA Chemical Assessment and Management Program (ChAMP)[3]. This chemical cluster was organized to maximize the potential information available to inform screening-level prioritization of chemicals needing further consideration and, where possible, to prioritize among multiple needs. Although most of the information considered relates to hazard, inferences about exposure that can be drawn from existing environmental fate and regulatory information have also been used, and information from the 2006 Inventory Update Reporting (IUR)[4] is included to inform exposure potential when it is available.

These screening-level hazard characterizations are technical documents intended to support subsequent decisions and actions by Office of Pollution Prevention and Toxics (OPPT). They provide a vehicle for public access to a concise assessment of the technical data on MPV chemicals and provide information previously not readily available to the public. The screening-level hazard characterizations, as the name indicates, do not evaluate the potential risks of a chemical or cluster of chemicals. This initial prioritization does not constitute a final Agency determination. Recommended actions may be considered by EPA in the future based on a relative judgment regarding one or more of the chemicals in comparison with others evaluated under this program, and in light of the uncertainties presented by gaps in the available data that may be determined to exist.

The purpose of organizing chemicals into structural clusters for this characterization was to maximize the number of potential analogs identified for the MPV chemicals, thus maximizing the potential data available to inform the MPV hazard characterizations. Organizing each chemical and associated data within a cluster will help assessors identify chemical trends, detect outlying estimates and measured data, facilitate read across, assist in weight of evidence approaches, and support identification of appropriate sub clustering. During the review of each cluster, assessors will likely determine endpoint specific subclasses depicting sets of compounds with potentially similar mechanistic or biological properties within the larger structural cluster. These endpoint specific sub clusters, breakpoints, and trends will be described within each section of the hazard characterization.

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[2] USEPA, U.S. Commitments to North American Chemicals Cooperation: http://www.epa.gov/hpv/pubs/general/sppframework.htm.
[3] USEPA, ChAMP information: http://www.epa.gov/champ/.
[4] USEPA, IUR Reporting information: http://www.epa.gov/oppt/iur/index.htm.

1. STRUCTURAL CLUSTER JUSTIFICATIONS

The alkyl phenols cluster consists of eight organic compounds containing a phenolic hydroxyl group substituted and substituted with branched hydrocarbon chains of at least five carbons. Six cluster members contains the hydrocarbon chain para to the hydroxyl group (phenol, 4-nonyl-, branched, 84852-15-3; phenol, 2(or 4)-sec-tetracosyl-, 233587-36-5; phenol, 2(or 4)-sec-hexacosyl-, 234446-37-8; phenol, 2(or 4)-sec-octacosyl, 234446-38-9; phenol, 2(or 4)-sec-triacontyl-, 234446-39-0; and phenol, 2,4-dimethyl-6-(1-methylpentadecyl)-, 134701-20-5), while two members have this substituent in the ortho position (phenol, 2-(1-methylpropyl)-, 89-72-5 and phenol, 2-nonyl-, branched, 91672-41-2). One cluster member, phenol, 2,4-dimethyl-6-(1-methylpentadecyl), 134701-20-5, also contains methyl groups in the 2- and 4-positions.

The following chemicals were reported in the 2006 IUR as being manufactured in or imported to the U.S. and are subject to this prioritization assessment:

CAS Registry Number	CA Index Name
91672-41-2	Phenol, 2-nonyl-, branched
134701-20-5	Phenol, 2,4-dimethyl-6-(1-methylpentadecyl)-
233587-36-5	Phenol, 2(or 4)-sec-tetracosyl-
234446-37-8	Phenol, 2(or 4)-sec-hexacosyl-
234446-38-9	Phenol, 2(or 4)-sec-octacosyl-
234446-39-0	Phenol, 2(or 4)-sec-triacontyl-

A number of the above chemicals have previously been reviewed in EPA's New Chemicals Program. The other chemicals included in this cluster are structural analogs used as supporting chemicals to help inform the hazard characterization (HC) and hazard-based prioritization (HBP) assessment.

2. PHYSICAL-CHEMICAL PROPERTIES (Table A)

Limited experimental values are available for the members of this cluster. Members are expected to be liquids under standard temperature and pressure conditions. The log of the octanol/water partition coefficients (log K_{ow}) range from 3.28 to 3.46 for members with 15 or fewer carbons. Estimates for those members with 24 or more carbons, range from 10.4 to 16.2; although these values are outside the range of the model used to make the estimates, it can be concluded that the log K_{ow} for these chemicals is high. There is also a discernable breakpoint for boiling point, vapor pressure, and water solubility. For lower molecular weight cluster members, the boiling points range from 224 to 310ºC and the vapor pressures from 0.000046 to 0.023 hPa. The water solubility is moderate for these members. For higher molecular weight members, the boiling points range from 420 to 560ºC and the vapor pressures from 4.1×10^{-13} to 2.4×10^{-8} hPa. The water solubility is negligible for these cluster members. Estimated and experimental pKas are in a relatively narrow range of 11 to 12 for all members of this cluster.

3. ENVIRONMENTAL FATE (Table A)

One member of this cluster, phenol, 2-(1-methylpropyl)- (89-72-5), is expected to have moderate mobility in soil and the others are expected to have low mobility. Although estimated Henry's Law Constants suggest volatilization of the alkylphenols from water is moderate, volatilization will be mitigated by the presence of suspended solids and the chemicals tendency to partition to organic carbon. The rate of atmospheric photooxidation for members of this cluster is considered moderate; however, fugacity modeling indicates that phenol, 2-(1-methylpropyl)- (89-72-5) will partition predominately to soil and water and to a lesser extent air and that the remaining members will partition primarily to soil and sediment. The members of this cluster are not expected to hydrolyze. Estimates indicate that that all members of this cluster have the potential to biodegrade aerobically under environmental conditions, although experimental and estimated data indicate that members will not be readily biodegradable. The alkylphenols in this cluster vary in their degree of branching which can affect the degree and rate of biodegradation. Therefore, although the cluster members are expected to have low persistence, some may be moderately persistent. Bioaccumulation potential is estimated to be low for all members of the cluster.

4. AQUATIC ORGANISM TOXICITY (Table B)

All members of this cluster fall in the ECOSAR phenols class. Experimental data for phenol, 2-(1-methylpropyl)- (89-72-5) indicates moderate acute toxicity to aquatic invertebrates. Experimental data for phenol, 4-nonyl-, branched (84852-15-3) indicates moderate acute toxicity to fish and a high acute toxicity to aquatic invertebrates and algae. Estimated data for phenol, 2-nonyl-, branched (91672-41-2) indicates high acute toxicity to fish and aquatic invertebrates and moderate acute toxicity to algae. Chronic toxicity for cluster members with log Kow values < 6 is estimated to be high for fish, moderate to high for aquatic invertebrates, and moderate for algae. Experimental data for phenol, 4-nonyl-branched corroborates the estimates of high chronic hazard potential for fish. Cluster members with estimated log K_{ow} values > 10 are estimated not to cause acute or chronic effects at saturation based on their very low water solubility.

5. HUMAN HEALTH TOXICITY (Table C)

The majority of the data for assessing the mammalian toxicity of this cluster are for the supporting chemicals, phenol, 2-(1-methylpropyl)- (89-72-5) and phenol, 4-nonyl-, branched (84852-15-3). Acute toxicity of the supporting chemicals following oral exposure (multiple studies available) is moderate to low. Available data for the supporting chemical, phenol, 2-(1-methylpropyl)- (89-72-5), also indicates low acute toxicity following dermal exposure and moderate acute toxicity following inhalation exposure (study summaries can be found in the HPV Hazard Characterization for the Alkylphenols Category[5]). Additional acute toxicity data (oral and dermal in rats) submitted to EPA for a member of this cluster indicates low toxicity; however, identifying the chemical and the submission in which the data were provided may be

[5] www.epa.gov/ChAMP

confidential business information (CBI) and therefore the data are not provided in Table C. Repeated oral dose studies for phenol, 4-nonyl-, branched (84852-15-3) and phenol, 2,4-dimethyl-6-(1-methylpentadecyl)- (134701-20-5) in rats also indicate moderate to low hazard potential for the cluster. Additional repeated-dose data (oral exposure in rats) submitted to EPA for a member of this cluster indicates moderate toxicity; however, identifying the chemical and the submission in which the data were provided may be confidential business information (CBI) and therefore the data are not provided in Table C. In a reproductive toxicity study in which rats were exposed orally to phenol, 4-nonyl-, branched (84852-15-3), reproductive effects occurred at doses indicating moderate hazard. A prenatal developmental toxicity study, also conducted with phenol, 4-nonyl-, branched (84852-15-3), showed low maternal systemic toxicity and no developmental effects. Data for two cluster members show eye and skin irritation in rabbits, but negative skin sensitization in guinea pigs. Additional data submitted to EPA for a member of this cluster indicates potential skin irritation and mild but transient eye irritation in rabbits. Data for this chemical also indicates it causes skin sensitization in guinea pigs; however, identifying the chemical and the submission in which the data were provided may be CBI and therefore the data are not provided in Table C. *In vitro* mutation assays conducted with phenol, 2-(1-methylpropyl)- (89-72-5) and phenol, 4-nonyl-, branched (84852-15-3) produced negative results in *Salmonella typhimurium, E. coli,* and V79 Chinese hamster cells. Phenol, 4-nonyl-, branched (84852-15-3) did not cause chromosome aberrations *in vivo*. Additional data submitted to EPA for a member of this cluster showed negative results for genotoxicity in a reverse mutation assay conducted with *Salmonella typhimurium and E. coli* both with and without activation; however, identifying the chemical and the submission in which the data were provided may be CBI and therefore the data are not provided in Table C. OncoLogic predicts a low potential for carcinogenicity for all members of this cluster.

6. OVERALL HAZARD CHARACTERIZATION SUMMARY (Table D)

- Persistence and Bioaccumulation: Available experimental and estimated data indicate persistence is low for the members of this cluster. Experimental and estimated data for seven members of the cluster indicate that bioaccumulation potential is low.

- Environment: Available experimental and estimated data indicate that the overall acute and chronic aquatic toxicity of the alkylphenols cluster is moderate to high for members with log K_{ow} values < 6. Members with estimated log K_{ow} values > 10 are predicted to have no effects at saturation.

- Human Health: Available experimental data indicate a low to moderate hazard potential for acute and repeated-dose toxicity. Data for phenol, 4-nonyl-, branched (84852-15-3) indicates a low potential for prenatal developmental toxicity and a moderate potential for reproductive toxicity. The cluster members are expected to cause skin and eye irritation. At least one cluster member is a skin sensitizer, but two are not. Experimental studies indicate that members of this cluster are not likely to be genotoxic. Members of this cluster are not predicted to be carcinogenic.

7. 2006 NON-CBI IUR INFORMATION

Phenol, 2,4-dimethyl-6-(1-methylpentadecyl)- (134701-20-5); phenol, 2-nonyl-, branched (91672-41-2): According to the 2006 Inventory Update Rule (IUR) submissions[6], these chemicals had aggregated production and/or import volume(s) in the United States between 10,000 and 500,000 pounds. No industrial processing and uses were reported in the IUR submissions for these chemicals. Additionally, no commercial and consumer uses were reported in the IUR submissions for these chemicals.

Phenol, 2(or 4)-sec-tetracosyl-(233587-36-5): According to the 2006 IUR submissions, this chemical had aggregated production and/or import volume(s) in the United States between 500,000 and 1 million pounds. Industrial processing and uses reported in IUR submissions for this chemical were claimed confidential. No commercial and consumer uses were reported in the IUR submissions for this chemical.

Phenol, 2(or 4)-sec-hexacosyl- (234446-37-8): According to the 2006 IUR submissions, this chemical had aggregated production and/or import volume(s) in the United States between 10,000 and 500,000 pounds. Industrial processing and uses reported in IUR submissions for this chemical were claimed confidential. No commercial and consumer uses were reported in the IUR submissions for this chemical.

Phenol, 2(or 4)-sec-triacontyl- (234446-39-0); phenol, 2(or 4)-sec-octacosyl- (234446-38-9): According to the 2006 IUR submissions, each of these chemicals had aggregated production and/or import volume(s) in the United States between 10,000 and 500,000 pounds. No industrial processing and uses were reported in the IUR submissions for these chemicals. Additionally, no commercial and consumer uses were reported in the IUR submissions for these chemicals.

8. REGULATORY AND RELATED INFORMATION SUMMARY

- All cluster members are listed on the TSCA Inventory. Five cluster members (134701-20-5, 233587-36-5, 234446-37-8, 234446-38-9 and 234446-39-0) are commenced premanufacture notification (PMN) substances indicating that their potential risks, based on specified uses, have been previously assessed by EPA's New Chemicals Program. One cluster member (134701-20-5) is also subject to a proposed TSCA section 5(a)(2) significant new use rule (SNUR).
- One cluster member (89-72-5) has had exposure limits recommended by NIOSH (REL) and ACGIH (TLV).
- EPA's New Chemicals Program has identified "phenols" as a category with a hazard concern of potential ecotoxicity for phenols with log K_{ow}s below 7.4 (acute) and ~9 (chronic).

[6] USEPA, 2006 Partial Updating of TSCA Chemical Inventory.

9. INITIAL PRIORITIZATION DECISION FOR:

CAS Registry Number	CA Index Name
91672-41-2	Phenol, 2-nonyl-, branched
134701-20-5	Phenol, 2,4-dimethyl-6-(1-methylpentadecyl)-
233587-36-5	Phenol, 2(or 4)-sec-tetracosyl-
234446-37-8	Phenol, 2(or 4)-sec-hexacosyl-
234446-38-9	Phenol, 2(or 4)-sec-octacosyl-
234446-39-0	Phenol, 2(or 4)-sec-triacontyl-

Rationale and Uncertainties Considered in Prioritization Decision:

- The five clusters members with estimated log K_{ow} values > 10 are estimated to have low acute and chronic aquatic toxicity. Estimated and measured data indicate that the overall acute and chronic aquatic toxicity for cluster members with log K_{ow} values < 6 is moderate to high. Therefore, information concerning uses and the frequency of releases to water and resultant exposures would be useful in determining the extent of potential concern for aquatic organisms.
- Available data indicates moderate repeated-dose and reproductive toxicity, and possible skin and eye irritation and skin sensitization. One cluster member (91672-41-2) has a vapor pressure above 1.3×10^{-6} hPa, and EPA experience has shown that worker exposure to vapors have been a concern for chemicals with vapor pressures above that value. Exposure-related information would be useful to more completely assess human health concerns for the cluster members.
- EPA's review of that cluster member (134701-20-5) in the New Chemical Program resulted in development of a proposed non-section 5e SNUR which defined any use leading to releases of water or lack of appropriate protection in the workplace as a new use requiring EPA notification. These regulatory decisions may be relevant for other cluster members.

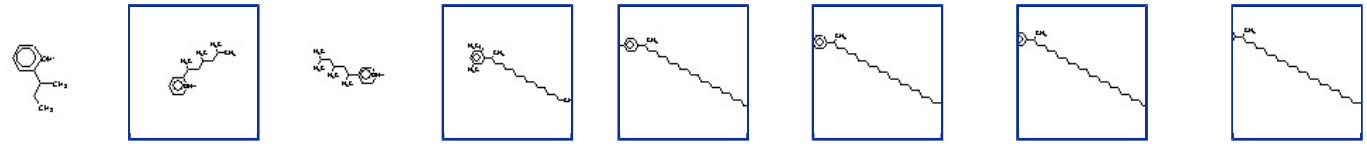
Prioritization Decision:

MEDIUM PRIORITY: consider whether concerns expressed in the SNUR proposed for one cluster member should be applied to other cluster members after reviewing use and exposure information for the one cluster member (91672-41-2) not reviewed in the New Chemicals Program.

- Recognizing the potential concerns for ecotoxicity and human health effects, the one cluster member (91672-41-2) not reviewed under the New Chemicals Program should be referred to the Interagency Testing Committee (ITC) as a candidate for the collection of exposure-related information and unpublished health and safety studies.
- EPA should evaluate the cluster members against the concerns expressed in the SNUR proposed under TSCA section 5(a)(2) for a cluster member (134701-20-5), and consider whether comparable (or other) actions may be needed for additional cluster members.

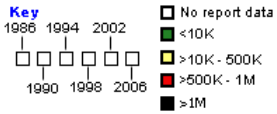
Table A **P-Chem Properties and Environmental Fate**

Alkyl phenols (8)



CASRN	89-72-5	91672-41-2	84852-15-3	134701-20-5	233587-36-5	234446-37-8	234446-38-9	234446-39-0
Chemical	Phenol, 2-(1-methylpropyl)-	Phenol, 2-nonyl-, branched	Phenol, 4-nonyl-, branched	Phenol, 2,4-dimethyl-6-(1-methylpentadecyl)-	Phenol, 2(or 4)-sec-tetracosyl-	Phenol, 2(or 4)-sec-hexacosyl-	Phenol, 2(or 4)-sec-octacosyl-	Phenol, 2(or 4)-sec-triacontyl-
Molecular Weight	150.22	220.36	220.36	346.6	430.76	458.82	486.87	514.93
Production Volume	■■■■■■	□□□■■□	■■■■■■	□□□□□□	□□□□□■	□□□□□□	□□□□□□	□□□□□□
State	Liquid		Liquid					
Melting Point (°C)	● 14		● 25					
Boiling Point (°C)	● 224	✧ 300	● 310	✧ 420	✧ 490	✧ 520	✧ 540	✧ 560
Vapor Pressure (hPa at 25°C	✧ 0.023	✧ 0.00034	● 0.000046	✧ 0.000000024	✧ 0.00000000012	✧ 0.000000000018	✧ 0.0000000000028	✧ 0.00000000000041
Water Solubility (mg/L)	✧ 1700	✧ 210	✧ 1400	✧ 0.00003	✧ 0.000000034	✧ 0.0000000033	✧ 0.00000000032	✧ 0.00000000003
log Kow	✧ 3.46	○ 3.28	● 3.28	✧ 10.4	✧ 13.3	✧ 14.3	✧ 15.3	✧ 16.2
Koc	✧ 2600	✧ 41000	✧ 40000	✧ 11000000	✧ 530000000	✧ 1800000000	✧ 6100000000	✧ 10000000000
pK_A/pK_B	✧ 11	✧ 11	● 11.06	✧ 12	✧ 12	✧ 12	✧ 12	✧ 12
HLC (atm-m^3/mole)	✧ 0.0000021	✧ 0.000017	✧ 0.000017	✧ 0.00015	✧ 0.0021	✧ 0.0042	✧ 0.0085	✧ 0.017
Hydrolysis								
Photolysis								
Photooxidation (half-life days)	✧ 0.24	✧ 0.21	✧ 0.21	✧ 0.25	✧ 0.15	✧ 0.14	✧ 0.14	✧ 0.13
Readily Biodeg	✧ No	✧ No	✧ No	✧ No	✧ No	✧ No	✧ No	✧ No
Rapid Biodeg	✧ Yes	✧ Yes	✧ Yes	✧ Yes	✧ Yes	✧ Yes	✧ Yes	✧ Yes
Ultimate Biodeg	✧ weeks	✧ weeks-months	✧ weeks-months	✧ weeks-months	✧ weeks-months	✧ weeks-months	✧ weeks-months	✧ weeks-months
Other Biodeg								
Other Fate								
Fugacity								
Air (%)	✧ 0.56	✧ 0.24	✧ 0.24	✧ 0	✧ 0	✧ 0	✧ 0	✧ 0
Water (%)	25	18	18	1.8	1.8	1.8	1.8	1.9
Soil (%)	74	81	81	30	30	30	30	30
Sediment (%)	0.69	0.76	0.76	68	68	68	68	68
BCF	● 16	✧ 67	✧ 67	✧ 3.2	✧ 3.2	✧ 3.2	✧ 3.2	✧ 3.2
BAF								

If no units provided - endpoint is unitless



Experimental

- ● Value from guideline study, clear weight of evidence, or evaluated database
- ■ Value from non-guideline but reliable experimental study
- ♦ Value reported without supporting details

Estimated

- ✧ Value from SAR/QSAR
- ○ Value obtained using read-across

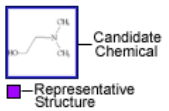
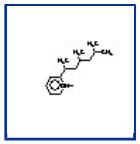
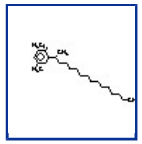


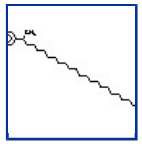
Table B

Alkyl phenols (8)

Aquatic Toxicity




CASRN	89-72-5	91672-41-2	84852-15-3	134701-20-5	233587-36-5	234446-37-8	234446-38-9	234446-39-0
Chemical	Phenol, 2-(1-methylpropyl)-	Phenol, 2-nonyl-, branched	Phenol, 4-nonyl-, branched	Phenol, 2,4-dimethyl-6-(1-methylpentadecyl)-	Phenol, 2(or 4)-sec-tetracosyl-	Phenol, 2(or 4)-sec-hexacosyl-	Phenol, 2(or 4)-sec-octacosyl-	Phenol, 2(or 4)-sec-triacontyl-
Molecular Weight	150.22	220.36	220.36	346.6	430.76	458.82	486.87	514.93
Production Volume	■■■■■■	□□□■■□	■■■■■■	□□□□□□	□□□□□■	□□□□□□	□□□□□□	□□□□□□
State	Liquid		Liquid					

ACUTE

Fish (mg/L)	**2.6** Freshwater fish 96h LC50 Phenols	**0.057** Freshwater fish 96h LC50 Phenols	**0.13** Pimephales promelas 96h LC50	**0.000034** (NES) Freshwater fish 96h LC50 Phenols	**0.00000035** (NES) Freshwater fish 96h LC50 Phenols	**0.000000072** (NES) Freshwater fish 96h LC50 Phenols	**0.000000015** (NES) Freshwater fish 96h LC50 Phenols	**0.0000000029** (NES) Freshwater fish 96h LC50 Phenols
Invertebrate (mg/L)	**1.3** Crangon septemspinosa 96h LC50 Phenols	**0.084** Daphnia magna 48h LC50 Phenols	**0.085** Daphnia magna 48h EC50	**0.0003** (NES) Daphnia magna 48h LC50 Phenols	**0.0000091** (NES) Daphnia magna 48h LC50 Phenols	**0.0000027** (NES) Daphnia magna 48h LC50 Phenols	**0.00000079** (NES) Daphnia magna 48h LC50 Phenols	**0.00000023** (NES) Daphnia magna 48h LC50 Phenols
Algae (mg/L)	**6.1** Green Algae 96h EC50 Phenols	**0.27** Green Algae 96h EC50 Phenols	**0.0563** Scenedesmus subspicatus 72h EC50	**0.0006** (NES) Green Algae 96h EC50 Phenols	**0.000014** (NES) Green Algae 96h EC50 Phenols	**0.0000038** (NES) Green Algae 96h EC50 Phenols	**0.000001** (NES) Green Algae 96h EC50 Phenols	**0.00000027** (NES) Green Algae 96h EC50 Phenols

CHRONIC

Fish (mg/L)	**0.004** Freshwater fish 60d ChV Phenols	**0.006** Freshwater fish 60d ChV Phenols	**0.014** Pimephales promelas 33d LOEC	**0.000034** (NES) Freshwater fish 30d ChV Phenols	**0.00000085** (NES) Freshwater fish 30d ChV Phenols	**0.00000023** (NES) Freshwater fish 30d ChV Phenols	**0.000000064** (NES) Freshwater fish 30d ChV Phenols	**0.000000018** (NES) Freshwater fish 30d ChV Phenols
Invertebrate (mg/L)	**0.28** Daphnia magna 21d ChV Phenols	**0.016** Daphnia magna 21d ChV Phenols	**0.024** Daphnia magna 21d NOEC	**0.000056** (NES) Daphnia magna 21d ChV Phenols	**0.0000017** (NES) Daphnia magna 21d ChV Phenols	**0.0000005** (NES) Daphnia magna 21d ChV Phenols	**0.00000015** (NES) Daphnia magna 21d ChV Phenols	**0.000000043** (NES) Daphnia magna 21d ChV Phenols

Algae (mg/L)	✧ 2.8	✧ 0.12	✧ 4.1	✧ 0.00025 (NES)	✧ 0.0000057 (NES)	✧ 0.0000015 (NES)	✧ 0.0000004 (NES)	✧ 0.00000011 (NES)
	Green Algae	Green Algae	Green Algae	Green Algae	Green Algae	Green Algae	Green Algae	Green Algae
	ChV	ChV	ChV	ChV	ChV	ChV	ChV	ChV
	Phenols	Phenols	Phenols	Phenols	Phenols	Phenols	Phenols	Phenols

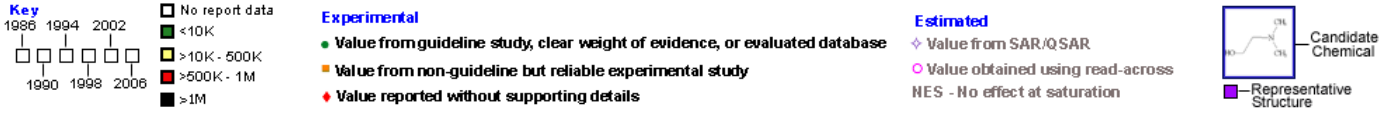
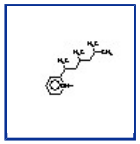
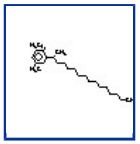
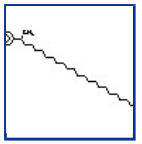


Table C **Human Health**

Alkyl phenols (8)




CASRN	89-72-5	91672-41-2	84852-15-3	134701-20-5	233587-36-5	234446-37-8	234446-38-9	234446-39-0
Chemical	Phenol, 2-(1-methylpropyl)-	Phenol, 2-nonyl-, branched	Phenol, 4-nonyl-, branched	Phenol, 2,4-dimethyl-6-(1-methylpentadecyl)-	Phenol, 2(or 4)-sec-tetracosyl-	Phenol, 2(or 4)-sec-hexacosyl-	Phenol, 2(or 4)-sec-octacosyl-	Phenol, 2(or 4)-sec-triacontyl-
Molecular Weight	150.22	220.36	220.36	346.6	430.76	458.82	486.87	514.93
Production Volume	■■■■■■	□□□■■□	■■■■■■	□□□□□□	□□□□□■	□□□□□□	□□□□□□	□□□□□□
State	Liquid		Liquid					
Acute	♦ **320** mg/kg o Rat		■ **1882** mg/kg o Rat					
Repeat Dose			■ L **150** mg/kg/day o Rat 90d	■ L **200** mg/kg/day o Rat 28d				
Reproductive			■ L **52.3** mg/kg/day o Rat 6w/pm/3 gen					
Developmental			■ L **150** mg/kg/day o Rat GD 6-15					
Genotoxicity	■ –		■ –					
Cancer	✧ –	✧ –	✧ –	✧ –	✧ –	✧ –	✧ –	✧ –
Eye Irritation			♦ **+** Rabbit					
Skin Irritation	■ **+** Rabbit		♦ **+** Rabbit					
Skin Sensitization			♦ – Guinea Pig					
Other Toxicity								

Key

1986 1994 2002 | 1990 1998 2006

□ No report data
■ <10K
■ >10K - 500K
■ >500K - 1M
■ >1M

Experimental
- ● Value from guideline study, clear weight of evidence, or evaluated database
- ■ Value from non-guideline but reliable experimental study
- ♦ Value reported without supporting details

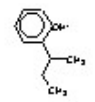
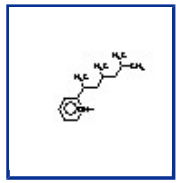
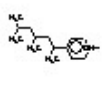
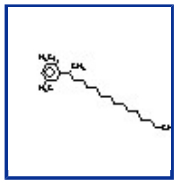
Estimated
- ✧ Value from SAR/QSAR
- ○ Value obtained using read-across

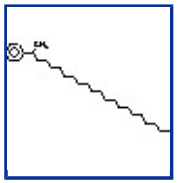
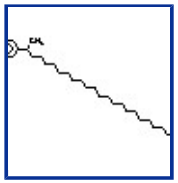
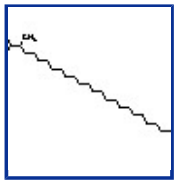
Route
O Oral
D Dermal
I Inhalation
X Other

Study Type
N NOAEL
L LOAEL
X Other

Table D
Alkyl phenols (8)

Overall Hazard Characterization

CASRN	**89-72-5**	**91672-41-2**	**84852-15-3**	**134701-20-5**	**233587-36-5**	**234446-37-8**	**234446-38-9**	**234446-39-0**
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Molecular Weight	150.22	220.36	220.36	346.6	430.76	458.82	486.87	514.93
Production Volume	■■■■■■	□□□■■□	■■■■■■	□□□□□□	□□□□□■	□□□□□□	□□□□□□	□□□□□□
State	Liquid		Liquid					
Environmental								
Persistence	✧ L	✧ L	✧ L	✧ L	✧ L	✧ L	✧ L	✧ L
Bioaccumulation	✧ L	✧ L	✧ L	✧ L	✧ L	✧ L	✧ L	✧ L
Aquatic Toxicity								
Acute	■ M	✧ H	■ H	✧ L	✧ L	✧ L	✧ L	✧ L
Chronic	✧ H	✧ H	■ H	✧ L	✧ L	✧ L	✧ L	✧ L
Human Health Effects								
Acute Toxicity	♦ M		■ L					
Repeated-Dose			■ L	■ M				
Reproductive			■ M					
Developmental			■ M					
Genotoxicity	■ –		■ –					
Cancer Hazard	✧ –	✧ –	✧ –	✧ –	✧ –	✧ –	✧ –	✧ –
Eye Irritation			♦ +					
Skin Irritation	■ +		♦ +					
Skin Sensitization			♦ –					

Key

1986 1994 2002
1990 1998 2006

□ No report data
■ <10K
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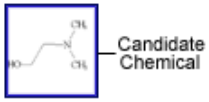
■ >1M



Experimental
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Estimated
- ✧ Value from SAR/QSAR
- ○ Value obtained using read-across

PCHEM/FATE	
Melting Point	
89725	USEPA-HPV-Hazard Characterization
84852153	USEPA-HPV-Hazard Characterization
Boiling Point	
89725	USEPA-HPV-Hazard Characterization
84852153	USEPA-HPV-Hazard Characterization
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233587365	EPI v3.2 2007
234446378	EPI v3.2 2007
234446389	EPI v3.2 2007
234446390	EPI v3.2 2007
Vapor Pressure	
89725	USEPA-HPV-Hazard Characterization
84852153	USEPA-HPV-Hazard Characterization
91672412	EPI v3.2 2007
134701205	EPI v3.2 2007
233587365	EPI v3.2 2007
234446378	EPI v3.2 2007
234446389	EPI v3.2 2007
234446390	EPI v3.2 2007
Water Solubility	
89725	EPI v3.2 2007
84852153	EPI v3.2 2007
91672412	EPI v3.2 2007
134701205	EPI v3.2 2007
233587365	EPI v3.2 2007
234446378	EPI v3.2 2007
234446389	EPI v3.2 2007
234446390	EPI v3.2 2007
Log Kow	
89725	USEPA-HPV-Hazard Characterization
84852153	USEPA-HPV-Hazard Characterization
91672412	Read-Across from 84852153
134701205	EPI v3.2 2007
233587365	EPI v3.2 2007
234446378	EPI v3.2 2007
234446389	EPI v3.2 2007
234446390	EPI v3.2 2007
Koc	
89725	EPI v3.2 2007
84852153	EPI v3.2 2007

91672412	EPI v3.2 2007
134701205	EPI v3.2 2007
233587365	EPI v3.2 2007
234446378	EPI v3.2 2007
234446389	EPI v3.2 2007
234446390	EPI v3.2 2007
pKa/pKb	
89725	SPARC Online Calculator v4.2
84852153	EFDB
91672412	SPARC Online Calculator v4.2
134701205	SPARC Online Calculator v4.2
233587365	SPARC Online Calculator v4.2
234446378	SPARC Online Calculator v4.2
234446389	SPARC Online Calculator v4.2
234446390	SPARC Online Calculator v4.2
Henry's Law Constant	
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84852153	EPI v3.2 2007
91672412	EPI v3.2 2007
134701205	EPI v3.2 2007
233587365	EPI v3.2 2007
234446378	EPI v3.2 2007
234446389	EPI v3.2 2007
234446390	EPI v3.2 2007
Photooxidation	
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84852153	EPI v3.2 2007
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134701205	EPI v3.2 2007
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234446378	EPI v3.2 2007
234446389	EPI v3.2 2007
234446390	EPI v3.2 2007
Ready Biodegradation	
89725	USEPA-HPV-Hazard Characterization
84852153	USEPA-HPV-Hazard Characterization
91672412	EPI v3.2 2007
134701205	EPI v3.2 2007
233587365	EPI v3.2 2007
234446378	EPI v3.2 2007
234446389	EPI v3.2 2007
234446390	EPI v3.2 2007
Rapid Biodegradation	

89725	EPI v3.2 2007
84852153	EPI v3.2 2007
91672412	EPI v3.2 2007
134701205	EPI v3.2 2007
233587365	EPI v3.2 2007
234446378	EPI v3.2 2007
234446389	EPI v3.2 2007
234446390	EPI v3.2 2007
Ultimate Biodegradation	
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84852153	EPI v3.2 2007
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134701205	EPI v3.2 2007
233587365	EPI v3.2 2007
234446378	EPI v3.2 2007
234446389	EPI v3.2 2007
234446390	EPI v3.2 2007
Fugacity	
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84852153	EPI v3.2 2007
91672412	EPI v3.2 2007
134701205	EPI v3.2 2007
233587365	EPI v3.2 2007
234446378	EPI v3.2 2007
234446389	EPI v3.2 2007
234446390	EPI v3.2 2007
BCF	
89725	Japan’s Ministry of Economy, Trade, and Industry’s MITI Biodegradation Database
84852153	EPI v3.2 2007
91672412	Read across from CASRN 84852-15-3.
134701205	EPI v3.2 2007
233587365	EPI v3.2 2007
234446378	EPI v3.2 2007
234446389	EPI v3.2 2007
234446390	EPI v3.2 2007
ECOTOXICITY	
Acute Fish	
89725	ECOSAR v.1.00
84852153	USEPA-HPV
91672412	ECOSAR v.1.00
134701205	ECOSAR v.1.00
233587365	ECOSAR v.1.00
234446378	ECOSAR v.1.00

234446389	ECOSAR v.1.00
234446390	ECOSAR v.1.00
Acute Daphnid	
89725	USEPA-HPV
84852153	USEPA-HPV
91672412	ECOSAR v.1.00
134701205	ECOSAR v.1.00
233587365	ECOSAR v.1.00
234446378	ECOSAR v.1.00
234446389	ECOSAR v.1.00
234446390	ECOSAR v.1.00
Acute Algae	
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84852153	USEPA-HPV
91672412	ECOSAR v.1.00
134701205	ECOSAR v.1.00
233587365	ECOSAR v.1.00
234446378	ECOSAR v.1.00
234446389	ECOSAR v.1.00
234446390	ECOSAR v.1.00
Chronic Fish	
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84852153	USEPA-HPV
91672412	ECOSAR v.1.00
134701205	ECOSAR v.1.00
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234446378	ECOSAR v.1.00
234446389	ECOSAR v.1.00
234446390	ECOSAR v.1.00
Chronic Daphnid	
89725	ECOSAR v.1.00
84852153	USEPA-HPV
91672412	ECOSAR v.1.00
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234446389	ECOSAR v.1.00
234446390	ECOSAR v.1.00
Chronic Algae	
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84852153	ECOSAR v.1.00
91672412	ECOSAR v.1.00
134701205	ECOSAR v.1.00

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234446378	ECOSAR v.1.00
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234446390	ECOSAR v.1.00
HUMAN HEALTH	
Acute Toxicity	
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Repeat Dose	
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134701205	USEPA-TSCATS section 8E
Reproductive	
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Developmental	
84852153	USEPA-HPV
Genotoxicity	
89725	USEPA-HPV
84852153	USEPA-HPV
Cancer	
89725	OncoLogic
84852153	OncoLogic
91672412	OncoLogic
134701205	OncoLogic
233587365	OncoLogic
234446378	OncoLogic
234446389	OncoLogic
234446390	OncoLogic
Eye Irritation	
84852153	USEPA-HPV
Skin Irritation	
89725	USEPA-HPV
84852153	USEPA-HPV
Skin Sensitization	
84852153	USEPA-HPV