PROPOSAL FOR IDENTIFICATION OF A SUBSTANCE AS A CMR, PBT, vPvB OR A SUBSTANCE OF AN EQUIVALENT LEVEL OF CONCERN

Substance name: Dodecylphenol (tested on Tetrapropenylphenol CAS No. 74499-35-7)

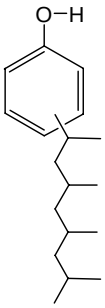
EC number: 248-312-8

CAS number: 27193-86-8

Registration number(s):

Molecular formula: $C_{16}H_{26}O$ to $C_{21}H_{36}O$

Structural formula:



idealised structure

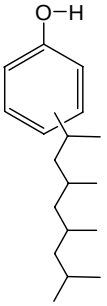
Summary of how the substance meets the CMR (Cat 1 or 2), PBT or vPvB criteria, or is considered to be a substance of an equivalent level of concern

The substance meets the T criteria, and is likely to meet the P (and vP) criteria (based on screening data). It does not meet the B criterion and so is not considered to be a PBT substance.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: Tetrapropenylphenol
EC Number:
CAS Number: 74499-35-7
IUPAC Name: Phenol (tetrapropenyl) derivatives
Molecular Formula: $C_{16}H_{26}O$ to $C_{21}H_{36}O$
Structural Formula:



idealised structure

Molecular Weight: 262.4 for idealised structure
Synonyms: TPP; dodecylphenol T

1.1 Purity/Impurities/Additives

1.2 Physico-Chemical properties

Table 1 Summary of physico-chemical properties

REACH ref Annex, §	Property	Value	Comments
V, 5.1	Physical state at 20 C and 101.3 KPa	Oily liquid	
V, 5.2	Melting / freezing point	-3°C	Pour point
V, 5.3	Boiling point		
V, 5.5	Vapour pressure	$9.2x10^{-3}$ Pa at 25°C	
V, 5.7	Water solubility	31 µg/l (main component) 2 mg/l (bulk substance)	
V, 5.8	Partition coefficient n-octanol/water (log value)	7.17	
VII, 5.19	Dissociation constant	>9.9	

2 MANUFACTURE AND USES

Not relevant.

3 CLASSIFICATION AND LABELLING

Classified as R50/53 by producer (classification inventory).

4 ENVIRONMENTAL FATE PROPERTIES

4.1 Degradation

4.1.1 Abiotic degradation

4.1.2 Biotic degradation

In a modified Sturm test ‘dodecylphenol T’ was added to a liquid mineral medium at concentrations of 10 and 20 mg/L, which was inoculated and aerated at a temperature of 21-23°C for 28 days. The inoculum used in the test was activated sludge from a municipal sewage plant and had a bacterial count of 3.3×10^4 CFU/ml (colony forming units per ml). The experiments were carried out without an emulsifier present. A positive control experiment was conducted using sodium benzoate. Degradation was monitored by measuring the actual CO_2 evolution compared with the theoretical

amount that would be evolved if the substance was completely oxidised. The control substance (sodium benzoate) achieved a degradation level of 95% within 28 days, reaching the threshold for ready biodegradability within 14 days. This indicated that the inoculum used had sufficient biological activity.

The substance achieved a degradation level of 25% at 10 mg/L and 6% at 20 mg/L within a period of 28 days. This result indicates that dodecylphenol is not readily biodegradable under the conditions of this test. The lack of biodegradation is unlikely to be a function of toxicity towards the bacterial culture, in view of the results reported in Section 4.1.6.

The low level of degradation observed in the ready biodegradability study could have been due to the poor availability of the substance to the micro-organisms in the test medium. Consequently, a study has recently been performed to investigate the inherent biodegradation potential of tetrapropenylphenol in aerobic aqueous conditions. The study was carried out in accordance with the draft OECD test guideline 302D (CONCAWE test), which has been specifically developed for use with poorly water soluble substances. The test material was prepared by applying a test solution in acetone to a glass fibre filter paper and evaporating the solvent (thereby increasing the surface area exposed to the micro-organisms), to give a test concentration of 24.3 mg/L, equivalent to 20 mg carbon/L. This was exposed to a composite microbial inoculum derived from soil and a waste water treatment plant (treating predominantly domestic sludge) in the dark for 56 days (following pre-exposure of the inoculum over 14 days to enhance its biodegradative potential). Degradation was determined by both carbon dioxide evolution and compound-specific analysis using HPLC. Abiotic test vessels were also prepared and analysed to correct for any losses of test material in the inoculated test vessels due to adsorption to glassware. A toxicity control was also included.

Based on carbon dioxide production, 10% degradation was achieved over 56 days. The results of compound specific analysis indicated that no significant chemical or biological degradation of the test material occurred. The toxicity control indicated that the test material was not toxic to the micro-organisms used in the study. Consequently, tetrapropenylphenol is not inherently biodegradable. It is interesting to note that the level of degradation was even lower than observed in the more stringent ready biodegradation test, but this might have been due to subtle differences in test substance composition.

4.1.3 Other information [1]

4.1.4 Summary and discussion of persistence

The results of biodegradation tests indicate that the substance is neither readily nor inherently biodegradable. The limited biodegradation observed in the two available studies is consistent with the branched structure of the substance.

4.2 Environmental distribution

4.2.1 Adsorption

[1] For example, half life from field studies or monitoring data

4.2.2 Volatilisation

4.2.3 Elimination in wastewater treatment plants

4.3 Bioaccumulation

4.3.1 Screening data[2]

4.3.2 Measured bioaccumulation data[3]

The bioconcentration of tetrapropenylphenol in rainbow trout (*Oncorhynchus mykiss*) was determined in a study to a protocol based on USEPA, ASTM and OECD guidelines (Wildlife International, 2006). Fish were exposed to two concentrations of tetrapropenylphenol (nominal levels 2 μg/L and 20 μg/L) in flow-through systems in stainless steel aquaria for a 27-day uptake period, which was followed by a 15-day depuration period. The environmental conditions (temperature, pH, dissolved organic carbon, hardness, alkalinity, conductivity, total organic carbon) were monitored throughout the test and were within acceptable limits.

The test substance used was a mixture of radiolabelled tetrapropenylphenol (uniformly ring-labelled) and non-labelled commercial material. The purity of both was 100% tetrapropenylphenol; the radiolabelled material contained 63% 14-C. (No analyses of the composition of the source materials were included.) Stock solutions were made up in dimethyl formamide (DMF). There was 0.1 mL/L of DMF in all exposures and in the solvent control.

The concentration of total radiolabel in the water was measured at intervals throughout the test by liquid scintillation counting; the mean measured concentrations on this basis were 1.1 μg/L and 11 μg/L for the uptake phase. A number of samples were also analysed by HPLC, with fluorescence detection, for different fractions (C_{5-10}, C_{11-12} and C_{13+}). The fraction that eluted before the C_{5-10} fraction was also measured and described as 'polar metabolites'. The sum of these four fractions was at least 75% of the concentration on the basis of total radioactivity in almost all samples. The concentrations are presented in Table 2.

Table 2 Mean measured substance concentrations in water during uptake phase

	Exposure series I 2 μg/L (nominal)		**Exposure series II 20 μg/L (nominal)**	
	Concentration (μg/L)	**% nominal**	**Concentration (μg/L)**	**% nominal**
Total radiolabel*	1.1	55	11	55
Polar metabolites*	0.06	-	0.51	-
C_{5-10}	0.21	11	2.1	11
C_{11-12}	0.51	25	5.2	26
C_{13+}	0.10	5	1.2	6

2 For example, log K_{ow} values, predicted BCFs

3 For example, fish bioconcentration factor

* Values not included in the study report, but derived from the data for this summary

Fish were sampled on days 0, 1, 3, 7, 11, 14, 21 and 24 of the uptake phase, and days 1, 3, 8 and 11 of the depuration phase. Two fish were taken at each time for the controls, and four for each exposure level. The fish were dissected into non-edible (head, fins and viscera) and edible tissues. The total radioactivity was determined in the individual samples by liquid scintillation counting. In addition, methanol extracts of pooled tissue samples (combining the four edible tissue samples at each time, etc.) were analysed by HPLC for the same four fractions as above. Again, the combined fractions gave a similar overall concentration to that determined on the basis of total radioactivity. The relative proportions of the four fractions in edible tissues were similar to those in water. In non-edible tissues, the proportion of polar metabolites was notably increased. The concentrations in fish did not increase further above the levels reached after three days at either exposure concentration. The steady state concentrations were taken as the mean of the measured concentrations over the period from 3 to 24 days. The concentrations are presented in Table 3, along with the concentrations of each of the fractions as determined by HPLC.

Table 3 Steady state concentrations in fish tissues (μg/kg wet weight)

	Nominal 2 μg/L			**Nominal 20 μg/L**		
	Edible	**non-edible**	**whole fish**	**edible**	**non-edible**	**whole fish**
Total radiolabel	317	1,762	905	3,184	15,707	8,237
Polar metabolites*	31.6	1,139	-	270	9,221	-
C_{5-10}	43.9	114	-	455	1,266	-
C_{11-12}	185	401	-	2,018	4,396	-
C_{13+}	42.6	98.7	-	508	1,123	-

* Values not included in study report, derived from data for this summary

A number of bioconcentration factor (BCF) values were derived from the above results. Values were calculated for the steady state concentrations based on the total radioactivity measurements for edible tissues, non-edible tissues and whole fish. Steady state values were also calculated for the individual fractions for edible and non-edible tissues. Values for whole fish by fractions were not calculated in the study report. Values have been estimated for this summary using the average ratio of edible:non-edible tissues at each exposure level; these were 1.46:1 for the 1.1 μg/L exposures and 1.49:1 for the 11 μg/L exposures. The concentrations at each sampling time in the uptake and depuration phases were used to calculate uptake and depuration rate constants, and hence kinetic BCF values. All of the BCF values are in Table 4.

Table 4 Bioconcentration factors

		1.1 μg/L exposure			**11 μg/L exposure**		
		edible	**non-edible**	**whole fish**	**edible**	**non-edible**	**whole fish**
Total radiolabel	- steady state	289	1,601	823	289	1,428	749
	- kinetic	328	1,787	920	329	1,611	844
C_{5-10}		209	544	345	217	603	372
C_{11-12}		362	786	534	388	845	572
C_{13+}		426	987	654	423	936	629

Note: Whole fish values for fractions calculated for this summary.

The study is considered to be valid. The metabolites were not identified, so it is not possible to conclude anything about their potential effects. As a result, the bioconcentration factor based on total radioactivity in whole fish is considered to be the most appropriate from this study. The steady

state values are preferred since they are based on direct calculation from the data rather than derived from data fitting, although in this case the kinetic values agree well. As a worst case the higher of the two steady state BCF values (823) is the preferred value from this study.

4.3.3 Other supporting information[4]

4.3.4 Summary and discussion of bioaccumulation

4.4 Secondary poisoning

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 HUMAN HEALTH HAZARD ASSESSMENT OF PHYSICOCHEMICAL PROPERTIES

Not relevant.

[4]For example, measured concentrations in biota

7 ENVIRONMENTAL HAZARD ASSESSMENT

7.1 Aquatic compartment (including sediment)

7.1.1 Toxicity test results

7.1.1.1 Fish

Acute toxicity

Long-term toxicity

7.1.1.2 Aquatic invertebrates

Acute toxicity

Long-term toxicity

A 21-day reproduction study has been carried out with *D. magna* in accordance with OECD test guideline 211. The test solutions were prepared using a stock solution of tetrapropenylphenol in acetone, and glassware was pre-conditioned with the appropriate test solution for approximately 24 hours prior to the initiation of the test to try to minimise the effects of adsorption. The test solutions were renewed three times per week. Concentrations were monitored analytically using HPLC at intervals throughout the study, following centrifugation at 40,000 g for 30 minutes. Based on nominal concentrations, a 21-d NOEC of 0.0037 mg/L, a 21-d LOEC of 0.012 mg/L and a 21-d EC_{50} for reproductive output of 0.0086 mg/L were found.

[In view of uncertainties over the actual exposure levels in the study, the results were re-calculated in the source document based on time-weighted means to give a 21-d NOEC of 0.0020 mg/L, a 21-d LOEC of 0.0027 mg/L (based on parental immobilisation and reproduction) and a 21-d EC_{50} for reproductive output of 0.0024 mg/L. These values are slightly lower than the nominal concentrations, but were preferred for the risk characterisation.]

7.1.1.3 Algae and aquatic plants

7.1.2 Sediment organisms

7.1.3 Other aquatic organisms

7.2 Terrestrial compartment

7.3 Atmospheric compartment

7.4 Microbiological activity in sewage treatment systems

7.5 Indirect exposure via the food chain

7.5.1 Effect data

8 PBT, vPvB AND EQUIVALENT LEVEL OF CONCERN ASSESSMENT

8.1 PBT, vPvB assessment

Persistence: the absence of any significant degradation in an inherent biodegradation test, which was designed to maximise degradation potential, implies that the substance would not degrade sufficiently quickly in a marine environmental simulation test to avoid meeting the persistence criterion. This is because although the test substance concentration would be much lower, the micro-organism population would be substantially less. The substance is therefore considered to be persistent, meeting the P (and potentially the vP) criterion, although this could be investigated further through simulation testing.

Bioaccumulation: a reliable *in vivo* experimental bioconcentration factor (BCF) of 823 has been measured for fish. Hence the substance does not meet the B (or vB) criterion.

Toxicity: the 21-day NOEC for *Daphnia magna* has been determined as 0.002 mg/L, and so the substance meets the T criterion.

Summary: tetrapropenylphenol is considered to clearly meet the T criterion, and is likely to meet the P and vP criteria with a reasonable degree of confidence. It does not meet the TGD B or vB criteria, and so is not considered a PBT substance according to the EU criteria.

8.2 Assessment of substances of an equivalent level of concern

INFORMATION ON USE, EXPOSURE, ALTERNATIVES AND RISKS

Not relevant as substance is not identified as a PBT.

OTHER INFORMATION

The information used in this report was taken from the following source:

Environmental Risk Evaluation Report: para-C_{12}-alkylphenols (Dodecylphenol and Tetrapropenylphenol). Environment Agency of England and Wales, 2006.