Australian Government

Department of Health and Aged Care Australian Industrial Chemicals Introduction Scheme

Di-tert-butylphenols

Evaluation statement (EVA00167)

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Draft



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AICIS evaluation statement (EVA00167)

Subject of the evaluation

Di-tert-butylphenols

Chemicals in this evaluation

Name	CAS registry number
Phenol, 2,6-bis(1,1-dimethylethyl)-	128-39-2
Phenol, 2,4-bis(1,1-dimethylethyl)-	96-76-4
Phenol, 2,5-bis(1,1-dimethylethyl)-	5875-45-6

Reason for the evaluation

Evaluation Selection Analysis indicated a potential environmental risk.

Parameters of evaluation

This evaluation considers the environmental risks associated with the industrial uses of three di-tert-butylphenols (DTBPs) listed on the Australian Inventory of Industrial Chemicals (the Inventory). In this evaluation the chemicals will be referred to as:

- phenol, 2,6-bis(1,1-dimethylethyl)- (2,6-DTBP)
- phenol, 2,4-bis(1,1-dimethylethyl)- (2,4-DTBP)
- phenol, 2,5-bis(1,1-dimethylethyl)- (2,5-DTBP).

These chemicals have been assessed for their risks to the environment according to the following parameters:

- Reported or default Australian introduction volumes of up to 100 tonnes per year (t/year).
- Industrial uses listed below in the 'Summary of introduction, use and end use' section.
- Potential emission into sewage treatment plants (STPs).

Summary of evaluation

Summary of introduction, use and end use

2,6-DTBP has a reported Australian introduction volume of up to 100 t/year. The default Australian introduction volume of 100 t/year is assumed for 2,4-DTBP and 2,5-DTBP. No specific information is available about the use and end uses of DTBPs in Australia.

Based on international use data, 2,6-DTBP and 2,4-DTBP predominantly have functional use as intermediates in the production of other higher molecular weight phenolic antioxidants. The chemicals are also used as antioxidants and/or stabilisers in the following products:

- fuel, oil, fuel oil additives and related products
- lubricant and grease products
- plastic and polymer products.

The chemical 2,6-DTBP is identified as an ingredient supporting the functionality and/or durability of fragrances.

Reported volumes from international jurisdictions indicate that 2,6-DTBP and 2,4-DTBP are used in the European Union (EU) at up to 10,000 t/year. The use volume in the United States of America (USA) is 45,359–453,592 t/year for 2,6-DTBP, and 4,536–45,359 t/year for 2,4-DTBP. There does not appear to be significant industrial use of 2,5-DTBP. As such, any uses of 2,5-DTBP are assumed to be consistent with the other DTBPs.

Environment

Summary of environmental hazard characteristics

Based on the information presented in this evaluation and according to the environmental hazard thresholds stated in the Australian Environmental Criteria for Persistent, Bioaccumulative and/or Toxic Chemicals (DCCEEW n.d.), all three DTBPs are:

- Persistent (P)
- Not Bioaccumulative (Not B)
- Toxic (T).

Environmental hazard classification

The DTBPs satisfy the criteria for classification according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) for environmental hazards as follows (UNECE 2017). This classification has been undertaken with the available data for 2,6-DTBP and 2,4-DTBP, which has been read across to 2,5-DTBP. This evaluation does not consider classification of physical and health hazards.

Environmental Hazard	Hazard Category	Hazard Statement
Hazardous to the aquatic environment (acute / short term)	Aquatic Acute 1	H400: Very toxic to aquatic life
Hazardous to the aquatic environment (long term)	Aquatic Chronic 1	H410: Very toxic to aquatic life with long lasting effects

Summary of environmental risk

DTBPs are categorised as persistent, not bioaccumulative, and toxic according to Australian categorisation criteria. They are used industrially as intermediates, antioxidants and stabilisers. As a result of their use pattern, these chemicals may be released to the aquatic environment in the treated effluent from sewage treatment plants. Exposure to sediment and soil is also possible via this pathway.

While categorised as persistent, monitoring data for DTBPs in jurisdictions with significantly higher introduction volumes than Australia indicates the presence of DTBPs in the environment is low. The predicted risk quotients for DTBPs in Australian surface waters, sediments, and soil are below the level of concern (RQs <1) based on international monitoring data and ecotoxicity test endpoints.

Conclusions

The Executive Director proposes to be satisfied that the identified risks to the environment from the introduction and use of the industrial chemicals can be managed.

Note:

- 1. Obligations to report additional information about hazards under *section 100* of the *Industrial Chemicals Act 2019* apply.
- 2. You should be aware of your obligations under environmental, workplace health and safety and poisons legislation as adopted by the relevant state or territory.

Supporting information

Rationale

This evaluation considers the environmental risks associated with the industrial uses of DTBPs. These chemicals are primarily used as intermediates in the production of higher molecular weight phenolic antioxidants. DTBPs are also used industrially as antioxidants or stabilisers in lubricants, plastics, rubber, fragrances, fuel, oil, and gasoline. These uses may result in environmental exposure through a common pathway involving release of the chemicals through treated effluents and biosolids produced by STPs.

The Evaluation Selection Analysis of DTBPs highlighted high production volumes for 2,6-DTBP and 2,4-DTBP internationally, and potential persistence and toxicity hazard characteristics. While significant industrial use of 2,5-DTBP has not been identified, and little hazard data is available, 2,5-DTBP has been included in this evaluation as its uses and hazards are expected to be analogous to the other DTBPs. This evaluation includes refinement of the risk characterisation of DTBPs and an in-depth assessment of the available environmental exposure and hazard information for these chemicals.

Chemical identity

CAS number	128-39-2
CAS name	Phenol, 2,6-bis(1,1-dimethylethyl)-
Molecular formula	C ₁₄ H ₂₂ O
Associated names	2,6-Di- <i>tert</i> -butylphenol
	2,6-DTBP
Molecular weight (g/mol)	206.32
SMILES (canonical)	OC=1C(=CC=CC1C(C)(C)C)C(C)(C)C
Structural formula	

CAS number

CAS name

Molecular formula

Associated names

Phenol, 2,4-bis(1,1-dimethylethyl)-

96-76-4

 $C_{14}H_{22}O$ 2,4-Di-tert-butylphenol

2,4-DTBP

206.32

Molecular weight (g/mol)

SMILES (canonical)

Structural formula

OC1=CC=C(C=C1C(C)(C)C)C(C)(C)C



CAS number	5875-45-6
CAS name	Phenol, 2,5-bis(1,1-dimethylethyl)-
Molecular formula	C ₁₄ H ₂₂ O
Associated names	2,5-Di- <i>tert</i> -butylphenol
	2,5-DTBP
Molecular weight (g/mol)	206.32
SMILES (canonical)	OC1=CC(=CC=C1C(C)(C)C)C(C)(

Structural formula



Additional chemical identity information

DTBPs are alkyl-substituted phenols. Impurities can include 2-tert-butylphenol (CAS RN 88-18-6, <0.5%) and 4-tert-butylphenol (CAS RN 98-54-4, <0.5%) (OECD 2002).

Relevant physical and chemical properties

Measured physical and chemical property data for 2,6-DTBP and 2,4-DTBP were retrieved from the database included in the OECD QSAR Toolbox (LMC 2020), the dossiers submitted under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation in the EU (REACH n.d.-a; REACH n.d.-b), and the OECD Screening Information Dataset (SID) initial assessment report (OECD 2002) for 2,6-DTBP. Most properties for 2,5-DTBP were calculated using EPISuite (US EPA 2017), while QSAR Toolbox was used to calculate the pKa values (LMC 2020).

The Henry's Law Constant values were calculated from the measured water solubility and vapour pressure values.

Chemical	2,6-DTBP	2,4-DTBP	2,5-DTBP
Physical form	Solid	Solid	Solid
Melting point	37°C (exp.)	56.8°C (exp.)	77°C (calc.)
Boiling point	253°C (exp.)	264°C (exp.)	281°C (calc.)
Vapour pressure	1.013 Pa at 20°C (exp.)	5.0 Pa at 38°C (exp.)	0.08 Pa at 25°C (calc.)
Water solubility	4.11 mg/L at 25°C (exp.)	33 mg/L at 25°C (exp.)	4.32 mg/L at 25°C (calc.)
Henry's law constant	50.86 Pa·m³/mol (calc.)	31.26 Pa⋅m³/mol (calc.)	3.82 Pa⋅m³/mol (calc.)
Ionisable in the environment?	No	No	No
рКа	11.7 (calc.)	11.6 (exp.)	10.6 (calc.)
log K _{ow}	4.5 at 24°C (exp.)	4.8 at 23°C (exp.)	5.3 at 25°C (calc.)

The pKa values indicate the phenolic functional group is unlikely to dissociate under normal environmental conditions (pH = 4-9). Similar physical and chemical properties are expected for 2,5-DTBP, as supported by EPI (Estimation Programs Interface) Suite calculations (US EPA 2017).

Introduction and use

Australia

The total volume of 2,6-DTBP introduced into Australia, reported under previous mandatory and/or voluntary calls for information, was up to 100 tonnes/year. The default Australian introduction volume of 100 t/year is assumed for 2,4-DTBP and 2,5-DTBP. No specific

information is available about the use and end uses of DTBPs in Australia. The use and end uses of DTBPs are assumed to be consistent with international uses.

International

The chemical 2,6-DTBP is on the United States (US) EPA High Production Volume list (US EPA 2020b) with annual use volumes of 45,359–453,592 tonnes (US EPA 2020a). 2,4-DTBP is also on the US EPA High Production Volume list (US EPA 2020b) with annual use volumes of 4,536–45,359 tonnes (US EPA 2020a). In the European Economic Area (EEA), 2,6-DTBP and 2,4-DTBP are registered for use in the range of 1,000–10,000 t/year (REACH n.d.-a; REACH n.d.-b).

Import and/or manufacture volumes for the di-alkyl phenols, including DTBPs, are reported to be between 7,000 and 40,000 tonnes per annum in Japan, for the period covering 2012–2020 (NITE 2020). In the Nordic countries, the average annual use volume over a 5 year period from 2016–2020 was 900 tonnes for 2,6-DTBP and 20.4 tonnes for 2,4-DTBP (SPIN n.d.). No specific international use volume data was located for 2,5-DTBP.

The main uses for DTBPs are as intermediates in the production of higher molecular weight phenolic antioxidants. Manufacturers in the US and Switzerland reported 75–95% and 95–100% of 2,6-DTBP produced is used as an intermediate in industrial processes, respectively (OECD 2002).

These chemicals (DTBPs) are also used as an antioxidant and stabiliser in fuel (NCBI n.d.; OECD 2002). The Consumer Product Information Database (CPID) reports concentrations of 2,6-DTBP up to 3% in fuel stabilisers (DeLima Associates n.d.). Use of 2,6-DTBP as an antioxidant has also been reported in lubricants, plastics and rubber (OECD 2002; REACH n.d.-b).

2,6-DTBP is identified as an ingredient supporting the functionality and/or durability of fragrances on the International Fragrance Association (IFRA) Transparency List (IFRA n.d.).

Existing Australian regulatory controls

Environment

The industrial uses of DTBPs are not subject to any specific national environmental regulations.

International regulatory status

United Nations

These chemicals (DTBPs) are not currently identified as persistent organic pollutants (UNEP 2001), ozone depleting substances (UNEP 1987), or hazardous substances for the purpose of international trade (UNEP & FAO 1998).

OECD

The chemical 2,6-DTBP was sponsored by Switzerland under the Cooperative Chemicals Assessment Programme (CoCAP). The Screening Information Data Set (SIDS) initial

assessment agreed 2,6-DTBP to be a low priority for further assessment, contingent on its use pattern as an intermediate and antioxidant remaining unchanged (OECD 2002).

Environmental exposure

The primary use of DTBPs as intermediates in the manufacture of phenolic antioxidants is not expected to be a significant environmental exposure pathway, as the parent compound is consumed during processing. Manufacturing activity and clean-up of equipment may lead to localised release of DTBPs in small quantities to wastewaters, soil, and air.

These DTBPs are also used as additive antioxidants in plastics and rubber. As DTBPs are not irreversibly bound within the polymer matrix for these applications, DTBPs may migrate to the surface of these materials and be released into the environment in small quantities from abrasion and wear during regular use.

The use of DTBPs in lubricants and fuels is expected to result in minimal environmental exposure, with correct disposal. A 2013 report found that only 4% of households were disposing of motor oil (either correctly or incorrectly) in Australia (Aither 2013). This suggests that Do it Yourself (DIY) users may make up a small portion of all consumers of vehicle maintenance products, and that most vehicle maintenance is performed through professional services. On this basis, the worst case exposure scenario arising from DIY uses would be a situation where all DIY users incorrectly disposed of lubricants and fuels containing the chemicals, estimated to be 4% of the volume used in lubricants and fuels. In the case of DTBPs, this is expected to be a very small fraction of the total introduction volume.

The chemical 2,6-DTBP is reportedly used in fragrance products to support the functionality and/or durability of an aroma compound (IFRA n.d.). End use products containing fragrances are typically released to wastewater as a normal part of their use. Depending on the efficiency of the degradation and partitioning processes in the STP, some fraction of the chemicals in wastewater entering STPs can be emitted to the air compartment, rivers or oceans in treated effluent, and to soil by application of biosolids to agricultural land (Struijs 1996).

Environmental fate

Partitioning

DTBPs are expected to partition to the soil, water, and sediment compartments when released into the environment from their industrial uses.

DTBPs are neutral organic chemicals, at environmentally relevant pH, that are slightly to moderately soluble in water and moderately volatile. The Henry's law constants indicate moderate volatility from water and moist soil. The measured sorption coefficient (K_{OC}) of 4,493 L/kg for 2,6-DTBP indicates that it will have only slight mobility in soil and will preferentially adsorb to phases in the environment with high organic carbon content (OECD 2002). Calculated K_{OC} values for 2,4-DTBP (9,010 L/kg) and 2,5-DTBP (9,010 L/kg) indicate immobility in soil (US EPA 2017).

Calculations with a standard multimedia partitioning (fugacity) model assuming release only to the water compartment (Level III approach) predict that 2,6-DTBP will mainly remain in water (64.7%) with some partitioning to sediment (34.5%), and minor quantities to air (0.75%) and soil (0.05%) (US EPA 2017). The predictions for 2,4-DTBP and 2,5-DTBP are similar (US EPA 2017).

Degradation

These DTBPs will undergo rapid primary degradation in water and air through photolytic mechanisms. However, DTBPs have demonstrated limited ultimate biodegradation in standard studies and may form persistent degradants in aqueous environments. Therefore, DTBPs are categorised as persistent.

The chemical 2,6-DTBP is not readily or inherently biodegradable in standard biodegradation tests. A study conducted in accordance with OECD Test Guideline (TG) 301B, reported 2,6-DTBP degradation across two test substance concentrations to be 5% (10 mg/L) and 1% (20 mg/L) theoretical carbon dioxide (ThCO2) within 28 days (REACH n.d.-b). An inherent biodegradation test (OECD TG 302C) conducted with 2,6-DTBP recorded 12–24% degradation, measured by biological oxygen demand (BOD), within 28 days (REACH n.d.-b).

The chemical 2,4-DTBP is not inherently biodegradable in standard biodegradation tests. A study conducted according to OECD TG 302C, reported negligible (0%) 2,4-DTBP degradation within 28 days. The test calculated oxygen uptake by percentage of calculated oxygen demand (% COD) and theoretical oxygen demand (% ThOD) (REACH n.d.-a). In a second test, 2,4-DTBP was evaluated for its biodegradability according to ISO Draft (BOD Test for Insoluble Substances). It attained negligible degradation (2%) within 28 days calculated from oxygen uptake (% ThOD) and therefore, cannot be considered as inherently biodegradable (REACH n.d.-a).

The chemical 2,6-DTBP undergoes rapid primary photodegradation in sunlit surface waters. A photolysis study conducted in accordance with US EPA OTS 795.70 measured 2,6-DTBP degradation by HPLC after sunlight irradiation for 29 hours in synthetic humic water and pure water. The overall photolysis half-life was calculated to be 2.41 hours (REACH n.d.-b).

A separate study observed 2,6-DTBP to undergo 71.31% degradation (10 mg/L to 2.87 mg/L) after 24 hours of irradiation. Control tests run without irradiation showed minimal degradation over the 24 hour test duration (Cui et al. 2019). The reported photolysis half-life for 2,6-DTBP was 11.382 hours. This study also observed that during the primary degradation of 2,6-DTBP via photolysis, it transformed into 2,5-DTBP. The same study reported 49.23% degradation of 2,4-DTBP after 24 hours of irradiation and suggested that the lower degradation rate was due to absorption of UV light. The reported photolysis half-life for 2,4-DTBP was 20.815 hours. The photodegradation products of 2,4-DTBP were not analysed in the study (Cui et al. 2019).

Another study reported the formation of 2,6-di-tert-butyl-p-benzoquinone (BHT-Q, CAS RN 719-22-2) as a degradant product of 2,6-DTBP under environmental conditions (Barber et al. 1999; Lopez-Avila 1981). BHT-Q has been shown to be stable under strong chlorination conditions, and this, along with likely recalcitrance to biodegradation, suggests it may persist in the environment (NICNAS 2020; Rodil et al. 2012).

These DTBPs are expected to undergo rapid photo-oxidation by hydroxyl radicals in the atmosphere with calculated half-lives of 1.4–2.6 hours (US EPA 2017). This is unlikely to be a significant dissipation pathway in the environment as DTBPs are only moderately volatile from water and have negligible partitioning to air.

Bioaccumulation

These DTBPs are not categorised as bioaccumulative in aquatic life, as the measured and predicted BCF values are below the Australian categorisation threshold value (BCF \ge 2000)

(EPHC 2009). Based on these studies and calculations, DTBPs are not categorised as bioaccumulative.

The measured octanol-water partition coefficients for 2,6-DTBP (log K_{OW} = 4.5) and 2,4-DTBP (log K_{OW} = 4.8), and the calculated value for 2,5-DTBP (log K_{OW} = 5.3), are above the domestic categorisation threshold for bioaccumulation hazards in aquatic organisms (log K_{OW} \geq 4.2), indicating a potential for bioaccumulation (EPHC 2009).

A study on 2,6-DTBP, with no test guideline stated, reported a BCF value of 660 L/kg in *Leuciscus idus melanotus* (Golden orfe) (REACH n.d.-b). A study, following OECD TG 305C, using 2,4-DTBP reported a BCF value of 436 L/kg in *Cyprinus carpio* (carp) (REACH n.d.-a; REACH n.d.-b). No bioaccumulation data were located for 2,5-DTBP; however, its calculated log K_{OW} (5.33) and BCF values (upper trophic with biotransformation = 846.5 L/kg) are similar to 2,4-DTBP and 2,6-DTBP.

Environmental transport

These DTBPs are not expected to undergo atmospheric long range transport based on their short half-lives in the atmosphere. DTBPs and their degradants may persist in water and have potential for long range transport in this compartment; however, no data has been identified to indicate this is the case.

Predicted environmental concentration (PEC)

The concentration of DTBPs in Australian river water, sediments, and soil are conservatively estimated to be 0.18 μ g/L, 56 μ g/kg dw and 0.74 μ g/kg dw, respectively. These values were determined by considering available international monitoring data for DTBPs in STP influents and effluents, biosolids, sediments, surface waters and biota.

The chemical 2,6-DTBP has been detected in international STP influents and effluents. In Sweden, influent concentrations ranged from 0.001–0.021 μ g/L and effluent concentrations were reported in the range of 0.0005–0.004 μ g/L (Hansen et al. 2008). A Swedish report by Paxeus (1999) cited in Remberger et al. (2003) found much higher levels of 25–145 μ g/L in incoming wastewaters, and 1.8–21 μ g/L in STP effluents. However, the reason for the elevated levels cannot be confirmed and they are inconsistent with contemporary measurements. Effluent concentrations ranging 0.06–0.17 μ g/L were found following secondary treatment at some locations in Chicago, Minneapolis/St. Paul, Detroit, Milwaukee, Des Plaines, and the Minnesota Rivers in North America (Barber et al. 1999).

International studies have quantified 2,6-DTBP in surface waters. The maximum value located in a range of studies was 0.18 μ g/L in the Minnesota Lakes, USA (Barber et al. 2012; Kolpin et al. 2002; Nantaba et al. 2021). The chemical has also been detected in surface runoff water and surface waters downstream from STPs at concentrations of <0.001–0.0649 μ g/L (Hansen et al. 2008).

Given its high production volume, 2,4-DTBP has also been detected frequently in rivers, lakes, and drinking water. Concentrations of 2,4-DTBP have been detected in surface waters in the nanogram to microgram per litre range (Liu et al., 2022). For example, in Laodao River in China, the concentration of 2,4-DTBP was observed as high as 300 μ g/L (Tang et al. 2015). However, insufficient information about the sampling location and potential sources of cross contamination was provided to validate this figure. (Tang et al. 2015) The highest surface water concentration measured in Sweden was 0.12 μ g/L (Remberger et al. 2003). Overall, the maximum observed value for 2,6-DTBP of 0.18 μ g/L in

international surface waters is taken as a PEC for surface waters in Australia, as it is conservative and typical of comparable international values.

A monitoring study in Sweden measured sediment concentrations of 2,6-DTBP at up to $9.0 \ \mu$ g/kg dw and 2,4-DTBP at up to $56 \ \mu$ g/kg dw in samples collected downstream from STPs (Remberger et al. 2003). The latter value has conservatively been used as the concentration of DTBPs in sediments in Australia for the purposes of risk characterisation.

Measured concentrations of 2,6-DTBP in biosolids retrieved from STPs in Nordic countries were reported in the range of $5.4-143 \mu g/kg dw$. This study also detected 2,6-DTBP in soil samples, but below the limits of quantification (Hansen et al. 2008).

The calculated 2,6-DTBP concentration in domestic soils amended with biosolids is $1.1 \ \mu$ g/kg dw based on the internationally measured biosolids concentration (143 μ g/kg dw), typical biosolids application rates and a soil bulk density of 1,300 kilograms per cubic metre (EPHC 2009).

Environmental effects

No ecotoxicity data are available for 2,5-DTBP. Due to structural similarity, read across from the available data for 2,6-DTBP and 2,4-DTBP has been used.

Effects on aquatic life

Acute toxicity

The following measured median lethal concentration (LC50) and median effective concentration (EC50) values for model organisms across three trophic levels were retrieved from the Registration Dossiers for 2,6-DTBP and 2,4-DTBP under the EU REACH legislation (REACH n.d.-a; REACH n.d.-b):

Taxon	Chemical	Endpoint	Method
Fish	2,6-DTBP	96h LC50 = 1.4 mg/L	<i>Pimephales promelas</i> (fathead minnows) OECD TG 204 Mortality Flow-through, measured
Invertebrate	2,6-DTBP	48h EC50 = 0.45 mg/L	Daphnia magna (water flea) US EPA TSCA TG Immobilisation Flow-through, measured
Invertebrate	2,4-DTBP	48h EC50 = 0.5 mg/L	Daphnia magna (water flea) OECD TG 202 Immobilisation Static, nominal
Algae	2,6-DTBP	96h EC50 = 1.2 mg/L	Raphidocelis subcapitata (green algae) US EPA TSCA TG 797.1050 Cell Number Static Measured concentration
Algae	2,4-DTBP	72h EC50 = 0.37 mg/L	Desmodesmus subspicatus (green algae) OECD TG 201 Growth rate Static Measured concentration

Chronic toxicity

The following measured no-observed-effect concentrations (NOEC) for model organisms across two trophic levels were retrieved from the Registration Dossiers for 2,6-DTBP and 2,4-DTBP under EU REACH legislation (REACH n.d.-a; REACH n.d.-b):

Taxon	Chemical	Endpoint	Method
Invertebrates	2,6-DTBP	21d NOEC = 0.035 mg/L	Daphnia magna (water flea) OECD TG 211 Reproduction and mortality Flow-through, measured
Invertebrates	2,4-DTBP	21d NOEC = 0.1 mg/L	Daphnia magna (water flea) OECD TG 211 Reproduction Flow-through, measured
Algae	2,6-DTBP	96h NOEC = 0.64 mg/L	Raphidocelis subcapitata (green algae) US EPA TSCA TG 797.1050 Cell number Static Measured concentration
Algae	2,4-DTBP	72h NOEC = 0.073 mg/L	Desmodesmus subspicatus (green algae) OECD TG 201 Growth rate Static Measured concentration

Effects on terrestrial life

The following measured NOEC and EC values for worms, terrestrial plants, and soil microorganisms exposed to DTBPs in soil were retrieved from the Registration Dossiers for 2,6-DTBP and 2,4-DTBP under EU REACH legislation (REACH n.d.-b):

Taxon	Chemical	Endpoint	Method
Worms	2,6-DTBP	56d NOEC = 51.44 mg/kg dw	<i>Eisenia fetida</i> (redworm) Reproduction OECD TG 222 nominal
Worms	2,4-DTBP	56d NOEC = 12 mg/kg dw	<i>Eisenia fetida</i> (redworm) Reproduction OECD TG 222 nominal
Terrestrial plants	2,6-DTBP	21d NOEC = 6.97 mg/kg soil dw	<i>Avena sativa</i> (oats) Shoot weight OECD TG 208 nominal
Terrestrial plants	2,4-DTBP	21d EC20 = 13.1 mg/kg soil dw	<i>Avena sativa</i> (oats) Shoot weight OECD TG 208 nominal
Soil microorganisms	2,6-DTBP	28d NOEC = 1000 mg/kg dw	Soil microorganisms Nitrate formation rate OECD TG 216 nominal
Soil microorganisms	2,4-DTBP	28d NOEC = 49.4 mg/kg dw	Soil microorganisms Nitrate formation rate OECD TG 216 nominal

Endocrine effects

Miller et al. (2001) determined the oestrogenic activity of a variety of phenolic additives by an in vitro yeast bioassay and reported submaximal (1/20,000,000th of estrogenic potency) oestrogenic activity for 2,6-DTBP. The study found that the main criterion for oestrogenic activity of alkylphenols is the presence of an unhindered phenolic (OH) group in a *para* position, whereas 2,6-DTBP and other DTBPs have a hindered OH group (Miller et al. 2001). An OECD Integrated Approaches for Testing and Assessment case study on the prediction of oestrogenic potentical of three target phenols incuding 2,4-DTBP concluded 2,4-DTBP, like other hindered phenols, is not expected to be potentially oestrogenic, whereas non-hindered phenols are potentially oestrogenic (Webster et al. 2019).

Predicted no-effect concentration (PNEC)

A freshwater PNEC for DTBPs of $3.5 \ \mu g/L$ was derived from the measured invertebrate chronic ecotoxicity endpoint (21d NOEC = $0.035 \ mg/L$) using an assessment factor of 10. This assessment factor was selected as reliable chronic and acute ecotoxicity data are available for the two most acutely sensitive trophic levels (EPHC 2009).

A calculated PNEC for sediment of 238 μ g/kg dw (EPHC 2009) was determined by the equilibrium partitioning method, using the water PNEC of 3.5 μ g/L, the measured K_{oc} of 4493 L/kg for 2,6-DTBP, and default values.

A soil PNEC of 697 μ g/kg soil dw for DTBPs was derived from the measured terrestrial plants chronic ecotoxicity endpoint (21d NOEC = 6.97 mg/kg dw) using an assessment factor of 10. This assessment factor was selected as reliable chronic ecotoxicity data are available for three trophic levels (EPHC 2009).

Categorisation of environmental hazard

The categorisation of the environmental hazards of the assessed chemical according to domestic environmental hazard thresholds is presented below:

Persistence

Persistent (P). Based on studies indicating incomplete ultimate degradation, DTBPs are categorised as Persistent.

Bioaccumulation

Not Bioaccumulative (Not B). Based on measured and predicted bioconcentration factors (BCF) in fish below 2000 L/kg, DTBPs are categorised as Not Bioaccumulative.

Toxicity

Toxic (T). Based on available acute and chronic ecotoxicity endpoints below 1 mg/L and 0.1 mg/L, respectively, DTBPs are categorised as Toxic.

Environmental risk characterisation

Based on the PEC and PNEC values determined above, the following Risk Quotients (RQ = PEC ÷ PNEC) have been calculated for release to surface waters, sediments, and soils:

Compartment	PEC	PNEC	RQ
Surface water	0.18 µg/L	3.5 µg/L	0.051
Sediment	56 µg/kg dw	238 µg/kg dw	0.235
Soil	1.1 µg/kg dw	697 µg/kg dw	0.0016

The main use of DTBPs as an intermediate will result in minimal environmental exposure. Other uses as an antioxidant and stabiliser in fuels, plastics, lubricants, rubber, and fragrances may result in limited releases to the environment via STPs. Following this release, DTBPs may end up in surface waters, sediment, and soil. However, predicted environmental concentrations for these compartments are relatively low based on international environmental monitoring. In terms of environmental hazards, DTBPs are categorised as persistent, not bioaccumulative and toxic. DTBPs demonstrate a lack of ultimate degradation and are categorised as persistent, they do not reach thresholds for categorisation as bioaccumulative and are acutely and chronically toxic in the aquatic compartment. While categorised as persistent, monitoring data for DTBPs in jurisdictions with significantly higher introduction volumes than Australia indicates the presence of DTBPs in the environment is low.

For sediment, soil, and surface waters, an RQ less than 1 indicates that DTBPs are not expected to pose a risk to the environment based on the predicted environmental concentrations being below the levels likely to cause harmful effects.

Uncertainty

This evaluation was conducted based on a set of information that may be incomplete or limited in scope. Some relatively common data limitations can be addressed through use of conservative assumptions (OECD 2019) or quantitative adjustments such as assessment factors (OECD 1995). Others must be addressed qualitatively, or on a case-by-case basis (OECD 2019).

The most consequential areas of uncertainty for this evaluation are discussed below:

- There are no Australian monitoring data for DTBPs. The risk profile of these chemicals may change should Australian monitoring data become available to indicate that these chemicals may be present in Australian surface waters, sediments, or soils at concentrations above the levels of concern.
- The categorisation of DTBPs as persistent is conservative in nature due to the lack of biodegradation observed in standard testing, and lack of evidence for complete mineralisation by abiotic degradation. If further evidence becomes available, it may change the persistence categorisation.
- There are no standard ecotoxicity data on sediment dwelling organisms available for DTBPs. The risk profile of this chemical may change should new ecotoxicity data or exposure data become available to indicate that DTBPs are present in Australian sediment above levels of concern.
- The identities and environmental effects of the degradation products of DTBPs in this evaluation are not fully evaluated. If more information becomes available in the future to indicate that these degradants may have persistent, bioaccumulative and toxic (PBT) characteristics, the PBT categorisation of DTBPs may change.

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