Annex 15 report

Proposal for identification of a substance of very high concern (SVHC)

2,4,6-Tri-*tert*-butylphenol

EC Number: 211-989-5

CAS Number: 732-26-3

November 2026

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List of abbreviations

B	Bioaccumulative
BAF	Bioaccumulation factor
BCF	Bioconcentration factor
BMF	Biomagnification factor
BOD	Biological oxygen demand
bw	Body weight
CAS	Chemical Abstracts Service
CREED	Criteria for reporting and evaluating exposure datasets
DUIN	Downstream User Import Notifications
dw	Dry weight
ECHA	European Chemicals Agency
EC	European Community
EU	European Union
GB	Great Britain
GC-MS	Gas chromatography – mass spectrometry
HLC	Henry's law constant
HPLC	High performance liquid chromatography
IOC	Ionizable Organic Chemicals
IUPAC	International Union of Pure and Applied Chemistry
K_{OA}	n-Octanol-air partition coefficient
K_{OW}	n-Octanol–water partition coefficient
MCL	Mandatory classification and labelling
MSC	Member State Committee
OECD	Organisation for Economic Cooperation and Development
P	Persistent
PBT	Persistent, bioaccumulative, and toxic
pK_a	Acid dissociation constant (logarithmic form)
REACH	Registration, Evaluation, Authorisation and restriction of Chemicals
SMILES	Simplified Molecular Input Line Entry System
STOT RE	Specific target organ toxicity – repeated exposure
SVHC	Substance of very high concern

TG	Test guideline
ThOD	Theoretical oxygen demand
Tpa	Tonnes per annum
UK	United Kingdom
vB	Very bioaccumulative
vP	Very persistent
ww	Wet weight

1 Proposal

Substance name: 2,4,6-Tri-*tert*-butylphenol

EC number: 211-989-5

CAS number: 732-26-3

2,4,6-Tri-*tert*-butylphenol, which is also known as 2,4,6-TTBP, has been identified as a substance of very high concern (SVHC) in accordance with the requirements set out in Annex 15 of EU REACH (ECHA, 2023b). This is owing to its classification in the hazard class toxic for reproduction category 1B (H360D: May damage the unborn child) and fulfilling the persistent, bioaccumulative, and toxic (PBT) criteria under Annex 13 of EU REACH (Regulation (EC) No 1907/2006.

This technical report provides an independent scientific assessment by the Agency[1] on whether 2,4,6-TTBP should be identified as an SVHC under UK REACH. The report only considers studies presented in the equivalent document produced by the European Chemicals Agency (ECHA), the EU Member State Committee (MSC) support document (ECHA, 2023a) unless stated otherwise. Relevant observations on studies made in the EU MSC support document have been summarised and Agency comments have been added where appropriate. The unpublished study reports were not available and have not been examined, unless stated otherwise. A targeted literature search was carried out for information to strengthen the biodegradation evidence for decision making (see Appendix A).

It is proposed to identify 2,4,6-TTBP as an SVHC according to Article 57(c) of UK REACH owing to its classification in the hazard class toxic for reproduction category 1B[2]. It is also proposed that 2,4,6-TTBP is identified as PBT according to Article 57(d) of UK REACH.

[1] The Health and Safety Executive (HSE) acting in its capacity as the Agency for UK REACH, and with support from the Environment Agency in accordance with Article 2B of UK REACH.

[2] Classification in accordance with section 3.7 of Annex 1 to the retained Regulation (EC) No 1272/2008 as amended for Great Britain (hereinafter referred to as GB CLP)

Summary of the assessment in relation to the criteria set out in Article 57 of the REACH Regulation

Toxic for reproduction – Article 57(c)

2,4,6-TTBP is identified as an SVHC in accordance with Article 57(c) owing to it being classified under GB CLP in the hazard class toxic for reproduction category 1B (H360D: May damage the unborn child).

Persistent, bioaccumulative and toxic – Article 57(d)

Persistence

2,4,6-TTBP screens as potentially persistent (P) and very persistent (vP) based on results from the BIOWIN v4.10 models of EPISuite™, and no or very low degradation in an OECD test guideline (TG) 301C ready biodegradability test and an OECD TG 306 biodegradability in seawater study. The Agency considers that the reliability of the studies is not assignable (Klimisch score 4) and so they can only be used as supporting evidence. However, the information is consistent with the finding that the substance was not inherently biodegradable in an OECD TG 302C study rated Klimisch 2 (‘reliable with restrictions’).

There is one non-standard simulation study available that has examined the degradation of 2,4,6-TTBP in seawater. The Agency rates the reliability of this study as Klimisch score 4, and so it can only be used as supporting evidence. The primary transformation half-life in seawater was 92 days after adjustment to 9°C, which is longer than the Annex 13 criterion for designation as P/vP (half-life > 60 days).

There is therefore a consistent weight-of-evidence of limited degradation potential from biodegradation modelling, ready biodegradability and biodegradability in seawater studies, inherent biodegradability testing, and a seawater degradation simulation study suggesting a half-life exceeding 60 days. Despite the uncertainties, as a minimum, 2,4,6-TTBP fulfils the P criterion of Annex 13 of UK REACH.

Bioaccumulation

2,4,6-TTBP screens as potentially bioaccumulative (B) for aquatic organisms as the experimental log K_{OW} value of 7.1 from an OECD TG 117 study exceeds the screening criterion (log K_{OW} > 4.5). In addition, 2,4,6-TTBP screens as potentially bioaccumulative in air-breathing organisms as the log K_{OW} value is 7.1 and estimated log K_{OA} value is 10.5 (criteria are > 2 and > 5, respectively).

The key piece of evidence is a non-standard flow-through study (Klimisch score 2) conducted to a Japanese guideline using *Cyprinus carpio* (Common Carp) that gave a range of bioconcentration factor (BCF) values from 4,320 to 23,200 L/kg and 4,830 to 16,000 L/kg at exposure concentrations of 1 and 10 µg/L, respectively. This is supported with data from a further non-standard experimental study that gave a BCF of 12,620 L/kg (calculated at 5% lipid content).

Based on the weight-of-evidence, 2,4,6-TTBP fulfils both the B and the very bioaccumulative (vB) criteria of Annex 13 of UK REACH (BCF > 2,000 and > 5,000 L/kg, respectively).

Toxicity

2,4,6-TTBP has a mandatory classification in accordance with GB CLP for toxicity for reproduction category 1B (H360D: May damage the unborn child) and specific target organ toxicity after repeated exposure (STOT RE) category 2 (H373: May cause damage to organs (Liver) through prolonged or repeated exposure). It therefore fulfils the T criterion of Annex 13 of UK REACH.

Conclusion

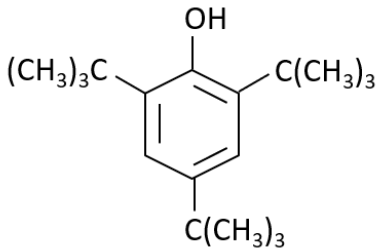
2,4,6-TTBP is proposed to be identified as a substance that meets the criterion of Article 57(c) of UK REACH owing to its classification in the hazard class toxic for reproduction category 1B. The Agency also proposes that 2,4,6-TTBP is identified as an SVHC on the basis of PBT properties according to Article 57(d).

2 Justification

2.1 Identity of the substance and physical and chemical properties

2.1.1 Name and other identifiers of the substance

Table 1: Substance identity

EC number:	211-989-5
EC name:	2,4,6-Tri-*tert*-butylphenol
SMILES[a]:	Oc(c(cc(c1)C(C)(C)C)C(C)(C)C)c1C(C)(C)C
CAS number:	732-26-3
IUPAC[b] name:	2,4,6-Tri-*tert*-butylphenol
GB Mandatory Classification and Labelling (MCL) List[c]:	604-097-00-6
Molecular formula:	$C_{18}H_{30}O$
Molecular weight:	262.43 g/mol
Synonyms:	2,4,6-TTBP
Structure:	

[a] SMILES: Simplified Molecular Input Line Entry System
[b] IUPAC: International Union of Pure and Applied Chemistry
[c] GB MCL list in accordance with the retained Regulation (EC) No 1272/2008 as amended for Great Britain

2.1.2 Composition of the substance

Substance type: mono-constituent

Table 2: Constituents other than impurities/additives

Constituents	Typical concentration
2,4,6-TTBP	≥ 80%

2.1.3 Identity and composition of transformation products relevant for the SVHC assessment

No transformation products were considered in ECHA (2023a). It is not necessary to consider transformation products since there are adequate data for 2,4,6-TTBP.

2.1.4 Identity and composition of structurally related substances (used in grouping or read-across approach)

No structurally related substances were considered in ECHA (2023a). It is not necessary to consider structurally related substances since there are adequate data for 2,4,6-TTBP.

2.1.5 Physicochemical properties

Physicochemical properties of 2,4,6-TTBP reported in ECHA (2023a) are summarised in Table 3. The source for all information was the EU REACH registration dossier (ECHA, 2018). All studies were conducted to GLP except for the estimated acid dissociation constant. The EU MSC support document made no comment on the reliability of the studies, except that all were rated as reliable without restrictions (Klimisch score 1) by the registrants.

Table 3: Overview of physicochemical properties of 2,4,6-TTBP

Property	Description/value	Method
Physical state at 20°C and 101.3 kPa	Slightly yellow powder	-
Melting/freezing point (°C)	131 (at 1,012 ± 1 hPa)	OECD TG 102
Boiling point (°C)	278 (at 1,012 ± 1 hPa)	OECD TG 103
Vapour pressure (Pa)	0.035 (at 20°C) 0.073 (at 25°C)	OECD TG 104
Density (kg/m^3 at 20°C)	0.977	OECD TG 109

Water solubility (mg/L at 20°C)	0.063	OECD TG 105
n-Octanol–water partition coefficient (log K_{OW})	7.1 (at 35°C and neutral pH)	OECD TG 117
Dissociation constant (pK_a)	12.62 (estimated value)	pKalc function of PALLAS estimation programme

Water solubility was determined using the column elution method of OECD TG 105 at two flow rates where equilibrium was established over more than 5 successive samples. The log K_{OW} value determined using OECD TG 117 (HPLC method) was beyond the range recommended by the method (0 to 6). However, the study included the reference substance benzo[ghi]perylene with a stated log K_{OW} of 7.2, so the test substance's log K_{OW} value fell within the range of the reference substances and no extrapolation was needed. There is no reason to contradict the reliability rating given to these studies. The Agency has not assessed the other studies of physicochemical properties.

The high pK_a value indicates that the substance will not be ionised at environmentally relevant pH values.

2.2 Mandatory classification and labelling

Table 4: Mandatory classification in the GB MCL list

Index number	International chemical identification	EC No	CAS No	GB MCL list classification		Aligned with EU CLH[a]
				Hazard class and category code(s)	Hazard statement code(s)	Y/N
604-097-00-6	2,4,6-Tri-*tert*-butylphenol	211-989-5	732-26-3	Repr. 1B Acute Tox. 4 STOT RE 2 Skin Sens. 1B	H360D H302 H373 (liver) H317	Y

[a]EU CLH is harmonised classification and labelling in accordance with Regulation (EC) 1272/2008.

2.3 Human health hazard assessment

Please see Section 2.2 (Mandatory classification and labelling).

2.4 Environmental fate properties

2.4.1 Degradation

2.4.1.1 Abiotic degradation

- Hydrolysis

ECHA (2023a) stated that no experimental data for hydrolysis were available and that there are no hydrolysable functional groups present in 2,4,6-TTBP. Hydrolysis is unlikely to be a relevant degradation route for 2,4,6-TTBP.

- Oxidation

No information on oxidation was reported in ECHA (2023a). 2,4,6-TTBP has the potential to undergo oxidation reactions since one of its uses is as an antioxidant. However, it has a highly branched chemical structure that hinders access to the phenol group, and it is unclear whether oxidation would occur under environmentally relevant conditions.

- Photochemical transformation

No information on photochemical transformation in the environment was reported in ECHA (2023a). The Agency estimated degradation in air using AOPWIN v1.92 model (EPISuite™ v4.10). Assuming 12 hours of daylight and a hydroxyl radical (OH) concentration of 1.5×10^6 OH/cm^3 the calculated half-life for 2,4,6-TTBP is 0.67 days. The hydroxyl radical rate constant is highly dependent on an assumed value for addition to an aromatic ring and therefore the reliability of this value is unclear.

2.4.1.2 Biodegradation

2.4.1.2.1 Biodegradation in the aqueous environment

2.4.1.2.1.1 Estimated data

ECHA (2023a) presented estimated biodegradation data from the BIOWIN v4.10 models of EPISuite™:

BIOWIN 2: 0.0068 (does not biodegrade fast)
BIOWIN 3: 2.0392 (ultimate degradation – months)
BIOWIN 6: 0.0130 (does not biodegrade fast)

The aromatic alcohol and carbon with four single bonds are fragments in the BIOWIN models that represent 2,4,6-TTBP well. The molecular weight of 2,4,6-TTBP is within the range of the substances used to derive the models and the datasets for all three models include several phenols including alkyl-substituted phenols. 2,4,6-TTBP is within the applicability domain of the three models.

ECHA (2023a) also discussed an assessment using Catalogic v5.12.1. Based on OECD TG 301C ready biodegradation tests (v10.14), the primary half-life for biodegradation was

171 days, and the half-life for ultimate biodegradation was greater than 10 years. ECHA (2023a) reported that 79% of fragments were within the applicability domain of the model and concluded that it was generally applicable to 2,4,6-TTBP. The Agency has not verified these values as it does not have access to this proprietary software but notes that the results are broadly consistent with the conclusions drawn from BIOWIN.

2.4.1.2.1.2 Screening tests

Three laboratory screening tests for 2,4,6-TTBP were presented in ECHA (2023a) and are summarised in Table 5.

Table 5: Summary of screening test results for 2,4,6-TTBP

Reference	Study type	Results
Lofthus *et al.* (2016)	64-day OECD TG 306 study using seawater amended with inorganic nutrients. 2,4,6-TTBP (5 mg/L) dispersed by ultra-sonication. Incubation at 20°C. Not assignable (Klimisch score 4)	Ultimate biodegradation: < 1% after 64 days
Unpublished (1981)	28-day OECD TG 301C study 2,4,6-TTBP at 30 mg/L Reference substance: aniline Incubation at 25°C Not assignable (Klimisch score 4)	Degradation: 2,4,6-TTBP: 0% based on biological oxygen demand, 5% based on HPLC (after 28 days) Aniline: 67% (after 7 days)
Unpublished (1992)	28-day OECD TG 302 study Inoculum: mixed population of activated sewage sludge micro-organisms (from 10 UK sites) 2,4,6-TTBP at 30 mg/L Aniline (100 mg/L) Reliable with restrictions (Klimisch score 2)	Degradation (based on oxygen consumption): 2,4,6-TTBP: max. of 17% (after 5 days) Aniline: 70% (after 14 days) 95% (after 28 days)

- Lofthus *et al.* (2016)

This study was reported to have been conducted according to OECD TG 306, although it is not stated whether it was the shake flask or closed bottle test. Seawater used as the test inoculum was collected from a depth of 80 m in a non-polluted Norwegian fjord (Trondheimsfjord). At the time of collection, the seawater had a salinity of 3.4%, a dissolved oxygen concentration of 8 mg/L, and a temperature of 6 to 8°C. Prior to testing, the seawater was acclimated to 20°C for 5 to 7 days and supplemented with inorganic nutrients as recommended in the guideline. 2,4,6-TTBP was applied at a nominal

concentration of 5 mg/L and dispersed by ultrasonication. This concentration was nearly 100-fold greater than the solubility of 2,4,6-TTBP (0.063 mg/L). Biodegradation was assessed as biological oxygen demand (BOD) expressed as a percentage of the theoretical oxygen demand (ThOD). Less than 1% ultimate degradation was observed after 64 days of incubation. The study report lacks detail, and consequently it is not possible to determine whether all validity criteria were met. The main limitations are summarised below:

- There are no details of procedural blanks, so no information on blank respiration is available.
- There is no information on reference substances so no assessment of the microbial activity of the seawater is possible.

In agreement with ECHA (2023a), the reliability of this study is not assignable (Klimisch score 4).

- Unpublished (1981)

This ready biodegradability study was conducted to OECD TG 301C. It was performed at 25°C with 30 mg of 2,4,6-TTBP added (no information on final concentration). Degradation after 28 days was 0% calculated from BOD and 5% from HPLC analysis. Degradation of the reference substance aniline was 67% after 7 days. The substance is not readily biodegradable based on this result. ECHA (2023a) stated that the substance remained undissolved at the end of the test. The reliability of this study is not known as it is not summarised in the EU REACH registration dossier, and the report is not publicly available. This study was also considered by the UK under OSPAR (OSPAR, 2006), where the same conclusion was drawn and lack of access to the full study report noted.

- Unpublished (1992)

This was a 28-day inherent biodegradability study conducted to OECD TG 302C (modified MITI Test (II)). The inoculum (100 mg dw/L) was a mixture of activated sewage sludge from ten different sites around the UK. The test substance was 2,4,6-TTBP (30 mg/L) and the reference substance was aniline (100 mg/L). The test was conducted in the dark at 25 ± 1°C and the solution agitated by a magnetic stirrer. Control and blank test systems were included. Percent degradation was determined by comparing BOD to ThOD, with oxygen consumption measured directly using a manometer. Degradation was corrected for blank values and reached a maximum of 17% after 5 days and then remained approximately unchanged for the rest of the study. Reference substance degradation was 42%, 70%, and 95% after 7, 14, and 28 days, respectively. The substance is not inherently biodegradable based on this result.

ECHA (2023a) considered the study was reliable with restrictions (Klimisch score 2). The test conditions complied with the test guideline and the Agency has no evidence to disagree with this reliability designation. The concentration of 2,4,6-TTBP was

approximately 500 times greater than the solubility limit in pure water and therefore the availability for degradation of the test substance may have been reduced in this study and could be a contributory cause of the lack of degradation seen.

2.4.1.2.1.3 Biodegradation studies (simulation tests)

One non-standard aquatic simulation study is included in ECHA (2023a). This is summarised in Table 6.

Table 6: Summary of aquatic simulation data

Reference	Study type	Results
Lofthus *et al.* (2016)	2,4,6-TTBP on adsorbents submerged in seawater. Incubation for 64 days at 20°C in the dark. Reliability not assignable (Klimisch score 4)	Degradation half-life: 32.3 days at 20°C 92 days at 9°C (calculated using the Arrhenius equation)

- Lofthus *et al.* (2016)

This study was run in parallel to the OECD TG 306 test noted in Section 2.4.1.2.1.2. Seawater was collected at a depth of 80 m from a non-polluted Norwegian fjord (Trondheimsfjord) and acclimatised to 20°C for 5 to 7 days. 2,4,6-TTBP was immobilised onto hydrophobic sorbents (tetrafluoroethylene and ethylene polymer) which were then submerged in 275 mL flasks of seawater. The flasks were then capped with no headspace. The amount on the sorbent added to each flask averaged approximately 21.7 µg and the concentration in seawater averaged approximately 79 µg/L. Flasks with test substance and sterilised seawater were included in the experiment. Flasks containing sorbent and seawater, but no test substance were included as controls. The flasks were incubated in the dark at 20°C and triplicate samples were collected after 0, 5, 14, 28, 42, and 64 days (no agitation). Sorbent and seawater were extracted and analysed separately for the test substance. The study reported a primary transformation half-life of 30.1 days for 2,4,6-TTBP 'immobilised on the adsorbent' and a half-life of 32.3 days for the combined transformation of 2,4,6-TTBP attached to the adsorbent and in the seawater'. There was no lag phase and < 1% degradation of 2,4,6-TTBP in the sterilised seawater. Two other alkylphenols were part of the study but were run as separate experiments. It is stated that some of the alkylphenols investigated in this study desorbed into the water phase (27 to 34% after 5 hours) but specific information for 2,4,6-TTBP is not available.

ECHA (2023a) converted the half-life of 32.3 days at 20°C to a marine temperature of 9°C using the Arrhenius equation and an activation energy (E_a) of 65.4 KJ/mole to give a temperature adjusted half-life of 92 days.

ECHA (2023a) rated the reliability of the study as not assignable (Klimisch score 4) and considered that it could only be used as supporting evidence because:

- There was no information on the formation or fate of any degradation products or the extent of mineralisation so no mass balance was available.
- The concentration of suspended particulate matter and organic carbon content was not provided.
- The use of the sorbent introduced some uncertainty.

The Agency agrees that the missing information and the use of adsorbent introduce uncertainty. It is not clear if there were any losses from adsorption to the test vessel or irreversible adsorption to suspended matter. Although biodegradation of 2,4,6-TTBP did occur, it is difficult to comment on the microbial activity of the seawater taken from a depth of 80 m as no reference substance was used in the study. The reliability of this study is therefore not assignable (Klimisch score 4) and can only be used as supporting evidence for persistence.

2.4.1.2.2 Biodegradation in soil

No information was reported in ECHA (2023a).

2.4.1.3 Field data

No information on the degradation of 2,4,6-TTBP in field studies was reported in ECHA (2023a). The Agency conducted a brief literature search for such data, but no relevant studies were located (Appendix A).

2.4.1.4 Summary and discussion of degradation

No definitive abiotic degradation data were available for the persistence assessment. 2,4,6-TTBP lacks hydrolysable functional groups and although it acts as an antioxidant in commercial products so is capable of oxidation reactions, no data are available to suggest that this is a relevant route of environmental degradation.

BIOWIN model predictions suggest that degradation will be slow. Degradation was ≤ 5% over 28 days in an OECD TG 301C ready biodegradability test (Klimisch score 4) and < 1% after 64 days in an OECD TG 306 biodegradability in seawater study (Klimisch score 4). An OECD TG 302C inherent biodegradability study (Klimisch score 2) showed limited degradation (maximum of 17% by ThOD after 5 days with no evidence of further degradation up to 28 days). Since inherent tests are performed under theoretically favourable conditions, a low degree of degradation provides evidence that a substance may be persistent in the absence of a simulation test.

There was one non-standard simulation study available that examined the degradation of 2,4,6-TTBP in seawater. As concluded by ECHA (2023a), it can only be used as supporting information given the uncertainties associated with the use of a sorbent, and

the lack of information on suspended matter and mass balance. The primary transformation half-life from this study was 92 days (adjusted to a temperature of 9°C).

2.4.2 Environmental distribution

2.4.2.1 Adsorption / desorption

An unpublished OECD TG 121 study (2015) in the EU REACH registration dossier determined a log K_{OC} value of 5.3. Eight reference substances were used with a log K_{OC} range from 1.26 to 5.63. The study was stated to be reliable without restrictions (Klimisch score 1), and there is no reason to doubt its reliability from the study summary available.

2.4.2.2 Volatilisation

The reported vapour pressure of 2,4,6-TTBP is 0.073 Pa (at 25°C), measured using OECD TG 104. The EU REACH registration dossier stated that the study is reliable without restrictions (Klimisch score 1). There is no reason to doubt its reliability from the study summary available.

Henry's law constant (HLC) values, estimated using HENRYWIN v3.21 in EPISuite™ v4.1, are 0.978 and 0.699 Pa/m^3/mole for the bond contribution and group contribution methods respectively. 2,4,6-TTBP is adequately represented by the bond contribution descriptions and there are a number of structurally similar substances in the chemical dataset used to derive the regressions for bond descriptions and correction factors. It is therefore likely to be within the model applicability domain.

The vapour pressure and HLC values indicate that there is a possibility of volatilisation of 2,4,6-TTBP from surfaces, including from water.

2.4.2.3 Distribution modelling

ECHA (2023a) presented modelling according to MacKay Level III, part of EPISuite™ v4.1, that showed if 2,4,6-TTBP is released to water, it will mostly partition to sediment, and when released to soil, it will mostly remain in the soil (see Table 7).

Table 7: Environmental distribution pattern according to MacKay, Level III modelling

Environmental compartment	Mass amount (%)		
	Equal release	Release to water	Release to soil
Air	0.292	0.0187	0.000105
Water (surface)	8.99	25.5	0.0153
Soil	64.5	0.0302	99.9
Sediment	26.2	74.4	0.0446

2.4.2.4 Field data

ECHA (2023a) reported several monitoring studies (summarised in Table 8) and did not comment on their reliability. The reliability of monitoring data is often overlooked in regulatory assessments and so this was assessed by the Agency using the Criteria for Reporting and Evaluating Exposure Datasets (CREED) reliability assessment framework (Merrington *et al.*, 2024). The study by Liu *et al.* (2015) was relevant, well reported and included all of the required information and some of the recommended data at the silver assessment level; it was considered 'usable with restrictions'. The three other studies all included details of sampling and analytical methods including detection limits. Remberger *et al.* (2003) included limited general method quality data while Hansson *et al.* (2008) and Konieczny *et al.* (2017) did not include recovery data. Overall, these three studies were well reported and although lacking some details, the data are 'usable with restrictions'.

Table 8: Summary of environmental field data for 2,4,6-TTBP

Reference	Study details	Results
Remberger *et al.* (2003)	National and regional monitoring programme in Sweden: Water (n = 37) Sewage sludge (n= 32) Sediment (n = 23) Air (n = 19)	Concentrations reported: Water: 0.000033 to 0.012 µg/L Sewage sludge: < 0.0001 to 0.15 µg/g Sediment: 0.01 to 3.5 ng/g dry weight (dw) Soil: < 0.0001 ng/g dw Air: < 0.01 ng/m^3
Hansson *et al.* (2008)	Göta Älv estuary, Göteborg, Sweden 3 sites Sediment (2 samples per site)	Sediment concentration (ng/g dw): Site 1: 0.21; < 0.1 Site 2 0.17; < 0.1 Site 3: < 0.1; < 0.1
Liu *et al.* (2015)	Wastewater treatment plants, China Sludge samples (n = 56)	Concentration (ng/g dw): Geomean: 98.1 Range: 9.28 to 1,700
Konieczny *et al.* (2017)	Screening programme in Norway Sludge samples (n = 2)	Concentration (ng/g dw): Siemmestad: 5 to 27 Hamar: 34 to 47

Monitoring data are available from the Environment Agency. The analytical method was gas chromatography-mass spectrometry (GC-MS), the data are semi-quantitative, and the sites are distributed throughout England and include rural and urban locations. The results are summarised in Table 9 for freshwater and groundwater. The data show a very low level of detection in freshwater and groundwater with a maximum concentration of 0.004 µg/L, which was below the formal limit of detection of the method (0.01 µg/L) .

Table 9: Environment Agency monitoring results for 2,4,6-TTBP in freshwater and groundwater

Year	Total analyses	Total detections	% detection	Total sites detected	Concentration (µg/L)	
					Min	Max
Freshwater						
2019	2,645	1	0.04	1	0.004	0.004
2020	606	2	0.33	2	0.001	0.001
2021	1,478	0	0.00	0	-	-
2022	1,259	0	0.00	0	-	-
Groundwater[a]						
2019	1,231	3	0.24	3	0.001	0.002
2020	201	2	1.00	2	0.001	0.001
2021	61	0	0.00	0	-	-
2022	28	0	0.00	0	-	-

[a] Groundwater quality monitoring network data

2.4.2.5 Summary of environmental distribution

The log K_{OC} value and Mackay Level III modelling indicate that 2,4,6-TTBP is likely to mostly partition to soil and sediment in the environment. Although 2,4,6-TTBP is detected in environmental samples, concentrations are generally low except in some sewage sludges. Data for Great Britain are very limited and not linked to specific sources, but the detection frequency was ≤ 1% in freshwater and groundwater samples in England, with reported concentrations also very low (maximum 4 ng/L).

2.4.3 Bioaccumulation

2.4.3.1 Bioaccumulation in aquatic organisms (pelagic & sediment organisms)

2.4.3.1.1 Screening data

The measured log K_{OW} value of 7.1 (see Table 3) indicates that 2,4,6-TTBP is potentially bioaccumulative (as it is > 4.5).

2.4.3.1.2 Predicted data

ECHA (2023a) did not present predicted bioaccumulation data so the Agency has considered two software packages.

Aquatic bioconcentration factor (BCF) values were predicted with the BCFBAF v3.02 model of EPISuite™ v4.11 using the experimental log K_{OW} value of 7.1. For the regression-based mode, the BCF is 7,130 L/kg ww (log BCF = 3.85). 2,4,6-TTBP is present in the training set for the BCFBAF prediction with an experimental value of 13,804 reported, along with a number of BCF for other alkyl-substituted phenols. For the Arnot-

Gobas model, the BCF is 4,382 L/kg ww (log BCF = 3.64), calculated for the upper trophic level, including biotransformation rate estimates.

The bioaccumulation estimation tool (BET) v1.03 within EAS-E-Suite v0.982 (ARC, 2026; accessed 16 April 2026) was also used to assess bioaccumulation potential. 2,4,6-TTBP is in the chemical information database of the tool, and the default chemical inputs were chosen except for log K_{OW}, water solubility, and vapour pressure where the values from Table 3 were added and selected. The aqueous exposure bioaccumulation prediction (laboratory) was 19,600 L/kg wet weight (ww) for freely dissolved substance and 8,390 L/kg for total substance in the aqueous phase. Field aquatic bioaccumulation predictions also indicate bioaccumulation potential with all bioaccumulation factor (BAF) values much greater than 10,000 L/kg whether based on freely dissolved (range 1.42×10^6 to 1.24×10^7) or total substance (range 2.50×10^5 to 1.37×10^6) in the aqueous phase. The BET report is presented in Appendix B.

2.4.3.1.3 Aquatic bioaccumulation data

Two aquatic bioaccumulation studies were discussed in ECHA (2023a), and are summarised in Table 10 with further details provided below the table. Both studies were also considered by the UK under OSPAR (OSPAR, 2006), where the same conclusions were drawn and lack of access to the full study reports noted.

Table 10: Summary of aquatic bioaccumulation studies

Reference	Study type	Results / comments
Unpublished report (1982)	Japanese Guideline 'Bioaccumulation study of chemicals in fish and shellfish' (Kanpogyo No. 5, Yakuhatsu No. 615, 49 Kikyoku No. 392) Aqueous exposure over 8 weeks using *Cyprinus carpio* (Common Carp) Reliable with restrictions (Klimisch score 2)	Exposure concentration (1 µg/L): BCF 4,320 L/kg (after 1 week) to 23,200 L/kg (after 4 weeks) Exposure concentration (10 µg/L): BCF 4,830 L/kg (after 2 weeks) to 16,000 L/kg (after 6 weeks)
Tadokoro and Tomita (1987)	Aqueous exposure of *C. carpio* (Common Carp) over 4 weeks (measured concentration of 2,4,6-TTBP 13.9 µg/L Reliable with restrictions (Klimisch score 2)	Normalised BCF values: 2,524 L/kg (1% lipid content) 12,620 L/kg (5% lipid content)

- Unpublished report (1982)

This flow-through study, conducted to a Japanese guideline, exposed *Cyprinus carpio* (Common Carp) to either 1 or 10 µg/L of 2,4,6-TTBP at 25 ± 1°C for 8 weeks (GLP status not specified). The fish had an average weight of 27.7 g and an average length of 10.3 cm at the start of the study and were acclimatised at 25°C for 14 days. The stock test solution was prepared by dissolving test substance (1 g) and the dispersant hydrogenated castor oil (HCO-40) (40 g) in acetone which was then distilled off and demineralised water added to make a 1 L solution at 1,000 mg/L. This solution was diluted so that the final exposure of the fish to 2,4,6-TTBP was either 1 or 10 µg/L. A summary of the original study (NITE, 2026) stated measured concentrations in the water from 0.582 to 0.664 µg/L for the low concentration and 5.67 to 7.05 µg/L for the high concentration and speculates that losses could have been due to volatilisation, uptake by fish, adsorption to fish, or adsorption to waste materials/excreta. Stock solutions were replaced daily and a special test system for volatile substances was used (no details provided). Final analysis of 2,4,6-TTBP was by GC-MS.

No abnormalities were observed in the fish during exposure. The BCF values determined in the study are reproduced in Table 11 and ranged from 4,320 to 23,200 (at 1 µg/L), and from 4,830 to 16,000 (at 10 µg/L). The average lipid content of the fish was reported as 4.5%. No details of how the BCF values or other results are calculated are presented in the EU REACH registration.

Given the age of this study and the limited reporting of certain methodological aspects, it does not fully meet current standards for a definitive bioaccumulation assessment (e.g. only 2 fish sampled at each time point). Nevertheless, the study was conducted under a recognised test guideline, employed measured aqueous concentrations that were below the water solubility limit, and generated BCF values above 2,000 L/kg from all samples. As such, the results are suitable as supporting evidence for the bioaccumulative properties of 2,4,6-TTBP. It is unlikely that the BCF values were lipid normalised as lipid normalised values would generally be slightly higher than those reported in Table 11, given the reported average lipid content.

Table 11: Summary of BCF values

Exposure concentration (µg/L)	Week				
	1	2	4	6	8
1	4,320 4,630	10,400 8,330	23,200 16,400	8,220 13,400	8,430 20,200 10,200
10	5,130 5,490	4,830 5,010	13,800 11,400	16,000 7,100	5,930 12,200

- Tadokoro and Tomita (1987)

This non-standard study investigated the dependence of experimental BCFs on the lipid content of fish (GLP status not stated). The test species was *C. carpio* (Common Carp) which were exposed to a nominal concentration of 20 µg/L 2,4,6-TTBP for 4 weeks. The measured concentration was 13.9 µg/L. There were three batches of fish, divided by lipid content. The general differences in lipid content during exposure were maintained by different feeding regimes and lipid contents in food. The lipid content of the fish varied from 1.5 to 9% and the corresponding BCFs varied from 5,000 to 20,000 L/kg. The study used regression analysis to determine a BCF normalised to a lipid content of 1% of 2,524 L/kg. ECHA (2023a) presented a recalculated BCF normalised to a lipid content of 5%, as stated in ECHA Guidance Chapter R.11 (ECHA, 2017); the 5% lipid normalised BCF is 12,620 L/kg. ECHA (2023a) acknowledged the inevitable uncertainty associated with applying a normalisation process twice, but pointed out that the BCFs for individual fish were greater than 5,000 L/kg (it was not specified how many BCF values of the more than 20 available exceeded this value). The study was rated as reliable with restrictions (Klimisch score 2) by ECHA (2023a). The Agency has not independently assessed this study but acknowledges that it provides supporting evidence of bioaccumulation.

2.4.3.1.4 Terrestrial bioaccumulation

The log K_{OW} of 2,4,6-TTBP is 7.1 and the estimated value for log K_{OA} using EPISuite™ v4.1; KOAWIN v1.10) is 10.5. These values are above the criteria for potential bioaccumulation in air-breathing organisms (log K_{OW} > 2 and log K_{OA} > 5) stated in ECHA Guidance Chapter R.11 (ECHA, 2017).

ECHA (2023a) discussed a toxicokinetic study by Takahashi and Hiraga (1983) where a single oral dose (up to 260 mg/kg bodyweight (bw) 2,4,6-TTBP) was administered to Sprague-Dawley rats (*Rattus norvegicus*). Maximum concentrations were reached in liver, kidney, and spleen within 1.5 and 6 hours and within 24 hours for adipose tissues. 2,4,6-TTBP was not detected in urine or faeces. After clearance from the blood, 2,4,6-TTBP was found in adipose tissue. It was not possible to derive an overall elimination half-life but ECHA (2023a) concluded that 2,4,6-TTBP accumulates in adipose tissue. The Agency agrees with this conclusion.

2.4.3.2 Summary and discussion of bioaccumulation

The experimental log K_{OW} value for 2,4,6-TTBP is 7.1, which indicates that the substance is potentially bioaccumulative in aquatic organisms (log K_{OW} > 4.5). Predicted BCF values above 2,000 L/kg are obtained from the BCFBAF v3.02 model of EPISuite™ v4.11 and the BET model v1.03 within EAS-E-Suite v0.982.

No standard studies conducted to OECD TG 305 are available to assess the aquatic bioaccumulation potential of 2,4,6-TTBP. However:

- An old flow-through study (unpublished, 1982) conducted to a Japanese guideline using *C. carpio* (Common Carp) gave BCF values ranging from 4,320 to 23,200 L/kg. It is

unlikely that these values were lipid normalised; given the reported lipid content of the fish (4.5 %), BCFs normalised to a 5% lipid content would be slightly higher. Although it does not fully meet the requirements of OECD TG 305, measured aqueous concentrations were below the water solubility limit, and BCF values were above 2,000 L/kg in all samples.

- A non-standard experimental study with *C. carpio* that investigated the dependence of bioaccumulation on lipid content resulted in a BCF of 12,620 L/kg at 5% lipid content.

The log K_{OW} value (> 2) and estimated log K_{OA} value of 10.5 (> 5) also suggest the potential for bioaccumulation in air-breathing organisms. A definitive conclusion cannot be drawn, but it is noted that 2,4,6-TTBP accumulated in the adipose tissues of rats administered a single oral dose.

2.4.4 Toxicity information

Given the human health hazard information summarised in Section 2.2, no further consideration has been given to ecotoxicity (ECHA, 2023a).

2.5 Conclusions on the SVHC properties

2.5.1 CMR assessment

2,4,6-TTBP is covered by the entry with Index number 604-097-00-6 in the GB MCL list and is assigned the hazard class toxic for reproduction category 1B (H360D: May damage the unborn child). Therefore, 2,4,6-TTBP satisfies the criterion in Article 57(c) of UK REACH.

2.5.2 PBT and vPvB assessment

2.5.2.1 Persistence

2,4,6-TTBP screens as potentially persistent (P) and very persistent (vP) based on results from the BIOWIN v4.10 models of EPISuite™, and no or very low degradation in an OECD test guideline (TG) 301C ready biodegradability test and an OECD TG 306 biodegradability in seawater study. The reliability of the studies is not assignable (Klimisch score 4) and so they can only be used as supporting evidence. However, the information is consistent with the finding that the substance was not inherently biodegradable in an OECD TG 302C study rated Klimisch score 2 (‘reliable with restrictions’).

There is one non-standard simulation study available that has examined the degradation of 2,4,6-TTBP in seawater (Klimisch score 4, only used as supporting evidence). The primary transformation half-life in seawater was 92 days after adjustment to 9°C, which is longer than the Annex 13 criterion for designation as P/vP (half-life > 60 days).

There is therefore a consistent weight-of-evidence of limited degradation potential from biodegradation modelling, ready biodegradability and biodegradability in seawater studies, inherent biodegradability testing, and a seawater degradation simulation study suggesting a half-life exceeding 60 days. Despite the uncertainties, as a minimum, 2,4,6-TTBP fulfils the P criterion of Annex 13 of UK REACH.

2.5.2.2 Bioaccumulation

2,4,6-TTBP screens as potentially bioaccumulative (B) for aquatic organisms as the experimental log K_{OW} value of 7.1 from an OECD TG 117 study exceeds the screening criterion (log K_{OW} > 4.5). In addition, 2,4,6-TTBP screens as potentially bioaccumulative in air-breathing organisms as the log K_{OW} value is 7.1 and estimated log K_{OA} value is 10.5 (criteria are > 2 and > 5, respectively).

The key piece of evidence is a non-standard flow-through study (Klimisch score 2) conducted to a Japanese guideline using *C. carpio* (Common Carp) that gave a range of bioconcentration factor (BCF) values from 4,320 to 23,200 L/kg or 4,830 to 16,000 L/kg at exposure concentrations of 1 and 10 µg/L, respectively. This is supported with data from a further non-standard experimental study that gave a BCF of 12,620 L/kg (calculated at 5% lipid content).

Based on the weight-of-evidence, the Agency concludes that 2,4,6-TTBP fulfils both the B and the very bioaccumulative (vB) criteria of Annex 13 of UK REACH (BCF > 2,000 and > 5,000 L/kg, respectively).

2.5.2.3 Toxicity

2,4,6-TTBP has a mandatory classification for toxicity for reproduction category 1B (H360D: May damage the unborn child) and STOT RE category 2 (H373: May cause damage to organs (Liver) through prolonged or repeated exposure). It therefore fulfils the T criterion of Annex 13 of UK REACH.

2.5.2.4 Overall conclusion

The Agency concludes that 2,4,6-TTBP fulfils the PBT criteria of Annex 13 of UK REACH. It is therefore proposed to identify 2,4,6-TTBP as an SVHC according to Article 57(d).

3 Information on use, exposure and alternatives

3.1 UK and EU REACH registration status and tonnage

The substance is registered with an aggregated tonnage of 10 to 100 tonnes per annum (tpa) under UK REACH.

A total of 50 Downstream User Import Notifications (DUINs[3]) have been submitted under UK REACH.

Under EU REACH, the substance is registered with an estimated aggregated tonnage of 100 to 1000 (three active EU registrants).

3.2 General description of uses and exposure

2,4,6-Tri-tert-butylphenol is used as an antioxidant and stabiliser in industrial applications including in fuels, lubricants and polymer materials. Information reported in EU REACH registration dossiers indicates that the substance is present as a component of multi-constituent substances rather than being manufactured or imported as the substance on its own.

Exposure and environmental release may occur during the formulation and use of mixtures and materials containing the substance (ECHA, 2023a).

3.3 Alternatives

No information on specific alternatives is available.

[3] GB-based companies who imported substances from EU-based suppliers before UK REACH became law on 1 January 2021 had no EU REACH registration obligations as they were classed as Downstream Users (DUs). As they are now importers from outside of GB, they may have registration obligations under UK REACH. However, a transitional measure allows former DUs to suspend the registration until one of three deadlines (depending on tonnage and hazard). Where the identity of these imported substances was known, they could be included in a Downstream User Import Notification (DUIN) submitted to the Agency.

References

ARC (2026). Eas-E-Suite. Available at: https://arnotresearch.com/eas-e-suite/

ECHA (2017). Chapter R.11: PBT/vPvB Assessment. *Guidance on Information Requirements and Chemical Safety Assessment.* European Chemicals Agency. Helsinki, Finland. https://data.europa.eu/doi/10.2823/128621

ECHA (2018). ECHA REACH registration for 2,4,6-tri-tert-butylphenol; last updated 2026. Available at: https://chem.echa.europa.eu/100.010.900/dossier-list/reach/dossiers/active?searchText=732-26-3

ECHA (2023a). Member State Committee support document for identification of 2.4.6-tri-*tert*-butylphenol as a substance of very high concern because of its toxic for reproduction (article 57(c)) and PBT (article 57(d)) properties. European Chemicals Agency. Available at: https://chem.echa.europa.eu/100.010.900/activities/svhcIdentification/fef9554fe3df1373dab48ac23aaea4b3?searchText=732-26-3

ECHA (2023b). Inclusion of substances of very high concern in the Candidate List for eventual inclusion in Annex XIV. Available: https://chem.echa.europa.eu/api-activity-list/v1/svhcIdentification/documents?name=fef9554fe3df1373dab48ac23aaea4b3_D(2023)8585-DC.pdf

Hansson, K., Kaj, L. & Brorström-Lundén, E. (2008). One-off survey of 2,4,6-tri-tert-butylphenol and short chained chlorinated paraffins in the Göta Älv estuary, Sweden. For Swedish Environmental Protection Agency. IVL Swedish Environmental Research Institute Ltd. IVL Report U2263. Available at: https://dvsb.ivl.se/dvss/pdf/SCCPbutylphenol.pdf

Konieczny, R. M., Henninge, L. B., Dalen, H., Grabic, R., Ferenčík, M., Bergqvist, P.-A., Lyngstad, E., *et al.* (2017). Screening programme 2016: Suspected PBT compounds. For The Norwegian Environment Agency. COWI AS. M-1063. Available at: https://www.miljodirektoratet.no/globalassets/publikasjoner/m1063/m1063.pdf

Liu, R., Song, S., Lin, Y., Ruan, T. & Jiang, G. (2015). Occurrence of synthetic phenolic antioxidants and major metabolites in municipal sewage sludge in China. *Environmental Science & Technology,* 49(4), 2073-2080. https://doi.org/10.1021/es505136k

Lofthus, S., Almås, I. K., Evans, P., Pelz, O. & Brakstad, O. G. (2016). Biotransformation of potentially persistent alkylphenols in natural seawater. *Chemosphere,* 156, 191-194. http://dx.doi.org/10.1016/j.chemosphere.2016.04.132

Merrington, G., Nowell, L. H. & Peck, C. (2024). An introduction to Criteria for Reporting and Evaluating Exposure Datasets (CREED) for use in environmental assessments. *Integrated Environmental Assessment and Management,* 20(4), 975-980. https://doi.org/10.1002/ieam.4899

NITE (2026). Substance information (CAS RN: 732-26-3): Test data (Bioaccumulation: aquatic/sediment). Available at: https://www.nite.go.jp/chem/jcheck/template.action?ano=28651&mno=3-0540&cno=732-26-3&request_locale=en

OSPAR (2006). OSPAR Commission 2003 (2006 Update): OSPAR background document on 2,4,6-tri-tert-butylphenol. *Hazardous Substances Series.* [274/2006]. Available at: https://www.ospar.org/documents?v=6977

Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC.: European Commission. Available at: http://data.europa.eu/eli/reg/2006/1907/2022-12-17

Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006 (Text with EEA relevance). European Commission. Available at: http://data.europa.eu/eli/reg/2008/1272/2026-05-01

Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006 (Text with EEA relevance). UK Government. Available at: https://www.legislation.gov.uk/eur/2008/1272/contents

Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC (Text with EEA relevance). UK Government. Available at: https://www.legislation.gov.uk/eur/2006/1907/contents

Remberger, M., Kaj, L., Palm, A., Sternbeck, J., Kvernes, E. & Brorström-Lundén, E. (2003). Screening tertiary butylphenols, methylphenols, and long-chain alkylphenols in the Swedish environment. For Swedish Environmental Protection Agency. IVL Swedish Environmental Research Institute Ltd. IVL Report B1594. Available at: https://www.diva-portal.org/smash/get/diva2:658065/FULLTEXT01.pdf

Tadokoro, H. & Tomita, Y. (1987). The relationship between bioaccumulation and lipid content of fish. QSAR in Environmental Toxicology – II. Proceedings of the 2nd International Workshop on QSAR in Environmental Toxicology, McMaster University,

Hamilton, Ontario, Canada: D. Reidel Publishing Company, Dordrecht, The Netherlands. Available at: https://link.springer.com/book/10.1007/978-94-009-3937-0

Takahashi, O. & Hiraga, K. (1983). Metabolic studies in the rat with 2,4,6-tri-t-butylphenol: a haemorrhagic antioxidant structurally related to butylated hydroxytoluene. *Xenobiotica,* 13(5), 319-326. https://doi.org/10.3109/00498258309052270

Appendix A: Literature search

A literature search was undertaken by the Agency in August 2026 to identify published information relevant to the assessment of environmental degradation of 2,4,6-TTBP. The keywords listed in Table B.1 were searched for in SCOPUS (https://www.scopus.com), PubMed (https://pubmed.ncbi.nlm.nih.gov/), and EBSCO (Environment Agency Search Facility) to maximise the number of records identified.

Table B.1 Literature search terms and number of hits

Search terms	Scopus	EBSCO	PubMed
2,4,6-Tri-tert-butylphenol AND biodegradation	3	123	10

The identified records were screened manually for relevance to this assessment based on the title and abstract. Articles identified as of potential interest were obtained and reviewed for relevance. Those that were found to be relevant are discussed in the appropriate sections of this report. Further articles that were not identified as part of the literature search have been included. These were sourced from references within the literature search articles and contained information relevant to this assessment.

The full list of records that were identified as relevant to this assessment are available on request. Those identified as relevant but not used in this evaluation have been highlighted in Table B.2 and an explanation given for their omission.

Table B.2 Publications not used in this report

Publication	Comment
Seller-Brison, C., Weissbach, F., Jorner, K., Scheringer, M., Fenner, K. (2026). Hazard assessment of antioxidants as contaminants of concern. *Environ. Sci. Technol. Lett.*, 13(4), 560–567. https://doi.org/10.1021/acs.estlett.5c01217	No new information
Zhao, F., Wang, P., Lucardi, R. D., Su, Z., & Li, S. (2020). Natural sources and bioactivities of 2,4-di-tert-butylphenol and its analogs. ***Toxins***, 12(1), 35. https://doi.org/10.3390/toxins12010035	Natural occurrence discussion – analogues not highly substituted.

Appendix B: BET v1.03 summary

The following is the summary report from BET v1.03 within EAS-E-Suite v0.982 for the bioaccumulation assessment of 2,4,6-TTBP.

Chemical Summary

Chemical assessed
CAS: 000732-26-3
Name: 2,4,6-tri-tert-butylphenol
Molar Mass (g/mol): 262.43
SMILES: Oc1c(cc(cc1C(C)(C)C)C(C)(C)C)C(C)(C)C
IOC Type: N

Partitioning at 25°C
Log K_{OW}: 7.1
Log K_{OA}: 9.695

Bioaccumulation Thresholds
BCF: Non B: < 2,000; B: > 2,000; vB: > 5,000

Screening Criteria
Screening criteria based on assumptions that octanol is a reasonable surrogate for biopartitioning to storage lipids are commonly used in bioaccumulation assessments to evaluate the potential of chemicals to bioaccumulate. For example, under European REACH legislation:

- A log K_{OW} > 4.5 indicates the possibility of a substance to accumulate in aquatic organisms.
- The combination of a log K_{OA} > 5 with a log K_{OW} > 2 indicates the possibility of a substance to accumulate in air-breathing organisms.

For Ionizable Organic Chemicals (IOCs) that are appreciably dissociated at system pH and for many surface active substances, log K_{OW} is not a valid screening criterion for assessing bioaccumulation potential. The sliders to the left allow one to consider various BCF, BAF and BMF thresholds that change colours in the BET output below highlighting when bioaccumulation values exceed the selected criteria.

Laboratory predictions

This section reports BET model predictions for representative laboratory organisms.

Aqueous Exposure Bioaccumulation Predictions

Organism	k1 (L-water/kg-ww/d)	kT (1/d)	BCF (L-total/kg-ww)	BCF (L-free/kg-ww)
Generic Lab Fish	2.97e+02	1.52e-02	8.39e+03	1.96e+04

- k1 (L-water/kg-ww/d): chemical uptake rate constant from water.
- kT (1/d): total (terminal) chemical elimination rate constant.
- BCF (L-total/kg-ww): bioconcentration factor referenced to the total chemical concentration in the water (freely dissolved (bioavailable) chemical + chemical sorbed to suspended matter).
- BCF (L-free/kg-ww): bioconcentration factor referenced to the freely dissolved (bioavailable) chemical concentration in the water.

Dietary Exposure Bioaccumulation Predictions

Organism	kD (kg/kg/d)	kW (kg/kg/d)	kT (1/d)	BMFL (kg-lw/kg-lw; Diet)	BMFA* (gut temperature) (activity/activity; Diet)	BMFA* (gut temperature) (activity/activity; Ingesta)	BMFL Growth Cor.(kg-lw/kg-lw; Diet)	BMFA* Growth Cor. (gut temperature) (activity/activity; Diet)
Generic Lab Fish	Generic Lab Fish	7.24e-03	0.00e+00	1.52e-02	1.43e+00	1.27e+00	1.27e+00	1.68e+00
Generic Lab Rat	Generic Lab Rat	5.40e-02	1.14e-01	5.58e+00	5.39e-03	6.52e-03	6.52e-03	5.39e-03

- kD (kg-diet/kg-ww/d): chemical uptake rate constant from diet.
- kW (L-water/kg-ww/d): chemical uptake rate constant from water.
- kT (1/d): total (terminal) chemical elimination rate constant.
- BMFL (kg-lw/kg-lw; Diet): biomagnification factor calculated on the chemical concentrations in the total lipids (adipose and membrane lipid) of the consumer and its diet.
- BMFA (activity/activity; Diet): biomagnification factor calculated on a chemical activity (or fugacity for neutral chemicals) basis.
- BMFA (activity/activity; Ingesta): biomagnification factor calculated on a chemical activity (or fugacity for neutral chemicals) basis and normalizes exposure from the total quantity of ingested chemical (diet and drinking water).

*These values are temperature dependent. Temperature correction in EAS-E Suite relies on the enthalpies of phase change. Assumed default enthalpies of phase change are provided in the chemical information tab. However, the use of chemical specific values would be recommended.

Field predictions

This section reports predicted B-metrics for field organisms and food webs

Field Aquatic Bioaccumulation Predictions

Organism	BAF (L-total/kg-ww)	BAF (L-free/kg-ww)
Zooplankton	1.57e+05	1.42e+06
Benthic_invertebrate	2.50e+05	2.25e+06
Aquatic_invertebrate	3.17e+05	2.86e+06
Planktivorous_fish	4.70e+05	4.24e+06
Benthivorous_fish	5.97e+05	5.38e+06
Omnivorous_fish	7.82e+05	7.04e+06

- BAF (L-total/kg-ww): bioaccumulation factor calculated as the ratio of the chemical concentration in the organism (COrg) and the total chemical concentration in the water (CWtotal) at steady-state as COrg/CWtotal.
- BAF (L-free/kg-ww): bioaccumulation factor calculated as the ratio of the chemical concentration in the organism (COrg) and the freely dissolved (bioavailable) chemical concentration in the water (CWfree) at steady-state as COrg/CWfree.

Field Biomagnification Predictions

Worm-Shrew-Owl

Organism	BMFL (kg-lw/kg-lw; Diet)	BMFA (activity/activity; Diet)	BMFA (activity/activity; Ingesta)
Soil Invertebrate	NA	NA	NA
Common Shrew	3.12e-02	4.17e-02	4.17e-02
Robin	6.42e-02	8.21e-02	8.21e-02
Barn Owl, Tawny Owl	6.08e-02	7.45e-02	7.45e-02

Caribou-Wolf

Organism	BMFL (kg-lw/kg-lw; Diet)	BMFA (activity/activity; Diet)	BMFA (activity/activity; Ingesta)
Caribou, deer	4.56e-03	6.47e-03	6.47e-03
Wolf	4.12e-02	4.44e-02	4.42e-02

Aquatic

Organism	BMFL (kg-lw/kg-lw; Diet)	BMFA (activity/activity; Diet)	BMFA (activity/activity; Ingesta)
Phytoplankton	NA	NA	NA
Zooplankton	9.89e-01	2.20e+00	2.20e+00
Filter feeder (mussel)	1.54e+00	2.17e+00	2.17e+00
Freshwater Drum	1.12e+00	1.23e+00	1.23e+00
Alewife (< 4 yr)	1.00e+00	1.11e+00	1.11e+00
Yellow Perch	1.10e+00	1.24e+00	1.24e+00
Trout	1.18e+00	1.35e+00	1.35e+00
EaGull	7.97e-02	8.49e-02	8.49e-02
Otter	2.78e-02	3.01e-02	3.01e-02
Seal	1.03e-02	1.26e-02	1.26e-02
Polar Bear	1.20e-01	1.14e-01	1.14e-01

Agricultural and far-field human

Organism	BMFL (kg-lw/kg-lw; Diet)	BMFA (activity/activity; Diet)	BMFA (activity/activity; Ingesta)
Trout	1.18e+00	1.35e+00	1.35e+00
Beef	2.06e-03	3.20e-03	3.20e-03
Dairy	2.06e-03	3.19e-03	3.19e-03
Chicken, Turkey	8.61e-03	1.22e-02	1.22e-02
Hen	8.72e-03	1.24e-02	1.24e-02
Pork	3.24e-03	5.02e-03	5.02e-03
Human	5.43e-03	6.10e-03	6.10e-03

Chemical input

Symbol	Parameter	Unit	Value	Warning	Input Type
Name	Chemical name		2,4,6-Tri-*tert*-butylphenol		User Input
CAS	Chemical abstract service registration number		000732-26-3		User Input
SMILES	SMILES notation		Oc1c(cc(cc1C(C)(C)C)C(C)(C)C)C(C)(C)C		User Input

M	Molar mass	g/mol	262.43		User Input
ChemFeature	Chem Feature		Default		User Input
Log KOW,N	log10 octanol-water partition ratio, neutral	L/L	7.1		User Input
Log KOA,N	log10 octanol-air partition ratio, neutral	L/L	9.695		User Input
BP	Boiling point	Celsius	278		User Input
MP	Melting point	Celsius	131		User Input
VP	Vapor pressure	Pa	0.035		User Input
WatSol	Water solubility	mg/L	0.063		User Input
BioHL - fish	Biotransformation half-life fish (@ 0.01kg)	Hours	1552.52		User Input
BioHL - mammal	Biotransformation half-life mammal (@ 70kg)	Hours	12.2		User Input
EnvHL - outdoor air	Degradation half-life outdoor air	Hours	24.07		User Input
EnvHL - surface water	Degradation half-life surface water	Hours	2356.94		User Input
EnvHL - sediment	Degradation half-life sediment/solid	Hours	21212.46		User Input
EnvHL - indoor air	Degradation half-life indoor air	Hours	48.14		User Input
EnvHL - soil	Degradation half-life soil	Hours	4713.88		User Input
Scaling Factor KPrW	Scaling Log KPrW, A	Unitless	1		User Input
Scaling Factor KPrW	Scaling Log KPrW, B	Unitless	1		User Input
IRT	Intake rate threshold	mg/kg-ww/d	0.0028		User Input
IEC	Internal effect concentration□	mmol/kg-ww	5e-07		User Input
iTTC	Internal Threshold of Toxicological Concern	nmol/L-Blood	0.1		User Input

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