Annex 15 Report
Proposal for identification of a substance of very high concern (SVHC)

O,O,O-triphenyl phosphorothioate (TPPT)

EC Number: 209-909-9

CAS Number: 597-82-0

July 2026

Contents

1. Proposal

Substance Name(s): O,O,O-triphenyl phosphorothioate (TPPT)

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O,O,O-triphenyl phosphorothioate (TPPT) 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, 2024a). This is based on the substance fulfilling the persistent, bioaccumulative and toxic (PBT) criteria under Annex 13 of EU REACH.

This technical report provides an independent scientific assessment by the Agency[1] on whether TPPT should be identified as an SVHC under UK REACH. It considers only studies presented in the equivalent document produced by the European Chemicals Agency (ECHA), the EU Member State Committee (MSC) support document (ECHA, 2024b). Relevant observations on studies made in the EU MSC support document have been summarised and Agency comments have been added where appropriate. Unpublished study reports were not available and have not been examined, unless stated otherwise. A literature search was not performed because the existing information is considered to be sufficient for decision making.

It is proposed to identify TPPT as PBT according to Article 57(d) of UK REACH.

Summary of how the substance meets the criteria set out in Article 57 of the REACH Regulation

A weight-of-evidence determination according to the provisions of Annex 13 of UK REACH has been used to identify TPPT as an SVHC based on the evidence presented in ECHA (2024b).

Persistence

TPPT did not fulfil the criteria for ready or inherent biodegradability and therefore is potentially persistent (P) and very persistent (vP). Although photodegradation in air is rapid (half-life of 4 hours), partitioning to air is predicted to be very low. The degradation DT_{50} from the aerobic mineralisation study conducted at 12 ± 2°C (Klimisch score 1) is much longer than the time of the study (61 days) and therefore much longer than the P and vP criteria of Annex 13 of UK REACH.

The Agency concludes from the evidence available that TPPT fulfils the P and vP criteria of Annex 13 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.

Bioaccumulation

TPPT screens as potentially bioaccumulative (B) and very bioaccumulative (vB) in aquatic organisms and air breathing organisms based on a minimum log K_{OW} of 4.79 and a predicted log K_{OA} value of 10.09. Estimated laboratory bioconcentration factor (BCF) values refined with predicted elimination half-lives using the BET assessment within EAS-E-Suite were 2,320 and 2,340 L/kg based on dissolved or total substance in the aqueous phase, respectively. The lipid normalised steady state BCF (BCF_{SSL}) from a flow-through bioaccumulation study using Common carp (*Cyprinus carpio*) and a measured TPPT test concentration of 0.0183 mg/L was calculated at each timepoint in the uptake phase where steady state was assumed to be reached. The mean value was 1,912 ± 420 L/kg with four out of eight values above 2,000 L/kg. The lipid normalised kinetic BCF (BCF_k) value was 2,112 L/kg when based solely on uptake data.

The Agency concludes from the evidence available that TPPT fulfils the B criterion of Annex 13 of UK REACH.

Toxicity

The most sensitive chronic ecotoxicity endpoint for TPPT was for *Oncorhynchus mykiss* (Rainbow trout) with 97-d EC_{10} values of 2.1 µg/L (larval survival) and 2.2 µg/L (overall survival) and a 97-d no observed effect concentration (NOEC) of 1.7 µg/L (post hatch survival). The NOEC is less than the threshold criterion of 0.01 mg/L (10 µg/L) stated in Annex 13 of UK REACH and therefore the Agency concludes that TPPT fulfils the T criterion.

Conclusion

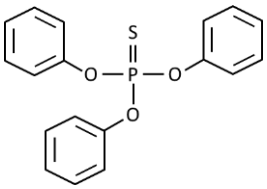
Based on the information available, the Agency concludes that TPPT fulfils the PBT criteria of Annex 13 of UK REACH and can therefore be identified as an SVHC in accordance with Article 57(d) of UK REACH.

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:	209-909-9
Substance name:	O,O,O-triphenyl phosphorothioate
SMILES[a]:	S=P(Oc1ccccc1)(Oc2ccccc2)Oc3ccccc3
CAS number:	597-82-0
IUPAC[b] name:	O,O,O-triphenyl phosphorothioate
Index number in GB Mandatory Classification and Labelling (MCL) List[c]:	No mandatory classification
Molecular formula:	$C_{18}H_{15}O_3PS$
Molecular weight range:	342.35 g/mol
Synonyms:	TPPT Phosphorothioic acid, O,O,O-triphenyl ester Triphenyl phosphorothioate Triphenyl thiophosphate Thiophosphoric acid triphenyl ester Triphenoxy(sulfanylidene)-lambda5-phosphane Tris(phenoxy)-sulfanylidenephosphorane
Structural formula:	

[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
O,O,O-triphenyl phosphorothioate	≥ 80% (w/w)

2.1.3 Identity and composition of degradation products/metabolites relevant for the SVHC assessment

No transformation products were considered in ECHA (2024b). The Agency has not considered transformation products as part of this assessment.

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 (2024b). The Agency has not considered any structurally related substances as part of this assessment.

2.1.5 Physicochemical properties

Physicochemical property information for TPPT summarised in ECHA (2024b) are presented in Table 3.

Table 3: Overview of physicochemical properties of TPPT presented in ECHA (2024b)

Property	Value
Physical state at 20°C and 101.3 kPa	Crystalline white solid
Melting/freezing point (°C)	~53
Boiling point (°C)	Decomposes at > 155 (first reaction) and > 255 (second reaction)
Vapour pressure (Pa at 20°C)	1.36×10^{-5}
Density (kg/m^3 at 20°C)	1,330
Water solubility (µg/L at 20°C)	20 ± 3 (pH 7)
n-Octanol–water partition coefficient (log K_{OW})	HPLC method (OECD TG 117): 4.79 (22°C; pH 6.7) 5 (23 °C; pH 6.4) Reported QSAR values from different models: 5.45, 5.98, 6.13, 6.33, 6.47

2.2 Mandatory classification and labelling

TPPT is not listed on the GB mandatory classification and labelling (MCL) list nor on Annex 6 of Regulation (EC) No 1272/2008.

2.3 Environmental fate properties

2.3.1 Degradation

Estimation data for hydrolysis and biodegradability potential reported in ECHA (2024b) have been excluded from the following sections because the relevant substances were not represented in the training or reference datasets, resulting in a high level of uncertainty in the generated values.

2.3.1.1 Abiotic degradation

The information on abiotic degradation presented in ECHA (2024b) is summarised in Table 4. TPPT was considered to be within the applicability domain of AOPWIN v1.92 as there were 12 organophosphate esters including six thiophosphate esters in the training dataset. Although the predicted half-life in air is 4 hours, the fugacity model of EPISuite™ predicts that partitioning to air will be low (< 0.1%).

Table 4: Summary of abiotic degradation data for TPPT presented in ECHA (2024b)

Abiotic degradation process	Information presented	Results
Hydrolysis	OECD TG 111 to GLP TPPT at 19 µg/L pH 4 and 7 (35 and 50°C) pH 9 (20, 35, and 50°C) Up to 30 days incubation Klimisch score 2	Half-lives for TPPT, extrapolated to 12°C using the Arrhenius equation: pH 4: 287 days pH 7: 278 days pH 9: 60 days
Oxidation	No data presented	-
Phototransformation	Estimated data using AOPWIN (v.1.92) Conditions: (12 hour day, OH radical concentration of 1.5 x 10^{-6} molecules/cm^3).	Phototransformation in air: Half-life is 4.0 hours

2.3.1.2 Biodegradation

2.3.1.2.1 Biodegradation in aqueous media

2.3.1.2.1.1 Screening tests

Two ready biodegradability and one inherent biodegradability test for TPPT are presented in ECHA (2024b). These are summarised in Table 5. Results from the two ready biodegradability studies (OECD TG 301B) indicate that TPPT is not readily biodegradable. Most of the validity criteria for the two studies were met and the Agency has no information to contradict the reliability score assigned in ECHA (2024b). The inherent biodegradability study (OECD TG 302B) was considered of unknown reliability (Klimisch 4) because the water solubility of TPPT is below that required by the guideline. Further to this, the study used radiolabelled TPPT, but no mineralisation measurements from radiolabelled carbon dioxide (CO_2) or mass balance are reported.

In addition, there were two studies carried out using the reaction mass of triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC no. 421-820-9), both given Klimisch score 2 in ECHA (2024b). The Agency has no information to contradict the reliability score assigned in ECHA (2024b). One study was conducted to OECD TG 301C using an inoculum made up of a mixture of sludge from ten different places in Japan. The other study was a closed-bottle OECD TG 301D test using a non-adapted domestic sludge-based inoculum. There was no mineralisation, measured by oxygen consumption, reported in either study.

The Agency concludes that TPPT is not readily or inherently biodegradable.

Table 5: Summary of screening test results for TPPT presented in ECHA (2024b)

Reference	Study details	Results
Unpublished study (1988)	28-day OECD TG 301B. Non-adapted domestic sewage TPPT at 10 or 20 mg/L Reference substance: aniline Klimisch score 2	Observed CO_2 evolution (28 days): 2% (10 mg/L TPPT) 0% (20 mg/L TPPT) 94.4% (aniline)
Unpublished study (2009)	29-day study conducted to OECD TG 301B. Dometic sludge inoculum ^{14}C-TPPT at 0.26 µg/L. Reference: sodium benzoate Klimisch score 2	Observed CO_2 evolution after 29 days: TPPT: 19.3% and 17.8% Sodium benzoate: 90.6% (14 days) TPPT present after 29 days (by HPLC): 51.5 and 60.8%
Unpublished study (2008)	28-day OECD TG 302B. Dometic sludge inoculum ^{14}C-TPPT at 0.26 µg/L Reference: ethylene glycol Klimisch score 4	Losses measured by liquid scintillation counting (LSC) after 28 days: TPPT: 59.5% and 66.8% Losses by DOC after 28 days: Ethylene glycol: 98.2% after 28 days

2.3.1.2.1.2 Simulation tests

ECHA (2024b) provides information on a Klimisch 1 (reliable without restriction) aerobic mineralisation study conducted to OECD TG 309 and to GLP. Results are summarised in Table 6.

Table 6: Summary of biodegradation simulation test results for TPPT presented in ECHA (2024b)

Reference	Study details	Results
Unpublished study (2021)	61-day OECD TG 309 study. Pond water and related sediment (at 20 mg/L) ^{14}C-TPPT (purity 97%; 2 and 10 µg/L) 12 ± 2°C in the dark Sampling after 0, 2, 7, 14, 21, 29, 45, and 61 days Klimisch score 1	TPPT > 90% of applied radioactivity (AR) at all timepoints (2 and 10 µg/L) Maximum of 4.0 and 4.3% CO_2 in any single sample ((2 and 10 µg/L) respectively First order dissipation rate constants: 6.8 x 10^{-15} d^{-1} (2 µg/L) 2.3 x 10^{-4} d^{-1} (10 µg/L)

- Unpublished report (2021)

The surface water and related sediment were sampled from a pond near Hanhofen, Germany. This was considered a suspended sediment test (suspended matter concentration of 20 mg/L). Nominal TPPT concentrations were documented as 2 or 10 µg/L applied in acetonitrile such that solvent concentration was 0.33%. Test vessels were aerated by gentle shaking with a constant flow of air. Radiolabelled sodium benzoate was used as the reference substance with acetonitrile added to 0.33%.

Mass balances exceeded 90% at all time points, with the exception of a single replicate at the 10 µg/L TPPT concentration, for which a value of 89% was recorded. TPPT accounted for approximately 90% of the applied radioactivity at all time points for both test concentrations. Carbon dioxide production did not exceed 4.0% and 4.3% of the applied radioactivity in any replicate at the low and high concentrations, respectively, and remained below 1% in the sterile control. Mineralisation of the reference substance, sodium benzoate, reached 83.4% after 14 days, demonstrating that the test system was biologically active.

ECHA (2024b) reports first-order kinetic rate constants of 6.8×10^{-15} d^{-1} and 0.00023 d^{-1} for the low and high concentrations respectively. These correspond to half-lives exceeding 800 days (lower limit of the 95% confidence interval) for both test systems. The Agency notes that these rate constants are not statistically different from zero and concludes that minimal degradation was observed over the 61-day study period. The Agency concludes that the study generally complies with OECD TG 309 and therefore agrees with the Klimisch score assigned. The Agency concludes that the degradation half-life is substantially greater than 61 days.

2.3.1.3 Summary and discussion of degradation

Abiotic degradation of TPPT by hydrolysis under environmental conditions is likely to be very slow. Although photodegradation in air is rapid (half-life of 4 hours), partitioning to air is predicted to be very low. TPPT did not fulfil the criteria for ready or inherent biodegradability and dissipation half-lives in freshwater from the aerobic mineralisation study conducted to OECD TG 309 (Klimisch score 1) were much longer than the length of the study (61 days). The Agency concludes that the degradation of TPPT under environmentally relevant conditions is likely to be slow.

2.3.2 Bioaccumulation

2.3.2.1 Bioaccumulation in aquatic organisms (pelagic & sediment organisms)

2.3.2.1.1 Screening information

Experimental and predicted log K_{OW} values reported for TPPT in ECHA (2024b), which are summarised in Table 3 are all greater than 4.5 and therefore TPPT screens as potentially B/vB.

2.3.2.1.2 Estimated data

The Agency used the BET assessment within EAS-E-Suite (ARC, 2026; accessed 16 April 2026) to investigate the bioaccumulation potential of TPPT. The results and supporting information are presented in Table 7 and Appendix A.

The aqueous exposure laboratory bioconcentration factor (BCF) predictions inclusive of the elimination half-life (HLB) in fish are above 2,000 for freely dissolved or total substance in the aqueous phase (2,430 and 2,450 L/kg, respectively). If HLB is not considered then these values exceed BCFs of 5000.

Field aquatic bioaccumulation predictions also indicate bioaccumulation potential with all bioaccumulation factors (BAFs) greater than 10,000 L/kg whether based on freely dissolved or total substance in the aqueous phase. Indicating that dietary exposure may be a significant uptake route. There was no indication of bioaccumulation from other field bioaccumulation predictions. All results considered are within the applicability domains of the models.

Table 7: Bioaccumulation Estimation Tool - 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 (inc. consensus HLB)	297	0.121	2,430	2,450
Generic Lab Fish (no HLB)	297	0.0057	5,160	5,210

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.

2.3.2.1.3 Aquatic bioaccumulation data

One aquatic bioaccumulation study is presented in ECHA (2024b). A summary of the study is presented in Table 8.

Table 8: Summary of aquatic bioaccumulation data for TPPT presented in ECHA (2024b)

Reference	Study details	Results
Unpublished study (1999)	Flow-through bioaccumulation study conducted to GLP. Test species: *Cyprinus carpio* (juvenile Common carp). Test substance: reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC no. 421-820-9) at 0.05 and 0.5 mg/L Klimisch score 2	For TPPT, steady state and lipid normalised BCF (BCF_{SSL}): 1,912 ± 420 L/kg (low exposure). 2,101 ± 594 L/kg (high exposure).

- Unpublished report (1999)

This was a bioaccumulation study conducted to GLP and following a Japanese guideline "Bioaccumulation test of a chemical substance in fish or shellfish" provided in "the Notice on the Test Method Concerning New Chemical Substances". The test species was *Cyprinus carpio* (Common carp) and study temperature 25.1 ± 0.6°C. At test initiation the fish weighed 26.4 ± 5.6 g and were 9.9 ± 0.6 cm long, with a measured lipid content of

4.3 ± 0.2%. The test substance was the reaction mass of triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC no. 421-820-9) applied at nominal concentrations of 0.5 or 0.05 mg/L using a hydrogenated castor oil-based hydrophilic emulsifier. The measured concentrations of TPPT in the dilution waters were 0.180 ± 0.002 and 0.0183 ± 0.0004 for 0.5 and 0.05 mg/L exposures concentrations, respectively. For each test concentration, 25 fish were used, with two individuals (labelled A and B) sampled at each uptake timepoint (days 7, 14, 21, 28, 42, and 56) and following 7 days of depuration. Water samples were collected concurrently with fish sampling, as well as on days 0 and 35.

The high test concentration (measured concentration of TPPT of 0.180 ± 0.002 mg/L) failed two of the validity criteria of OECD TG 305:

- The test concentration exceeded the water solubility of TPPT by a factor of around 10 (0.02 ± 0.003 mg/L at 20°C). It was noted that the highest concentration of hydrophilic emulsifier used was 1 mg/L
- All fish exhibited abnormal swimming behaviour from day 1, characterised by retrograde swimming movements and occasional convulsions. These symptoms persisted throughout the depuration period, with no evidence of recovery.

All validity criteria were passed for the low test concentration. The Agency notes that the study is broadly similar those conducted to OECD TG 305 but that sampling of two fish per sampling point is below the guideline recommendation of a minimum of four fish. Both concentrations were above the determined NOEC and EC_{10} values determined in a chronic fish study, although the Agency notes that the test species and life stage tested were different from that used in this study.

Reported TPPT concentrations in fish increased until week 3 of exposure and then remained approximately constant for the next four weeks, reaching a mean concentration of 30.4 ± 6.6 mg/kg (low concentration) and 323 ± 92 mg/kg (high concentration). An apparent steady state was therefore assumed. Water and fish concentrations and the resulting steady-state bioconcentration factor (BCF_{SS}) are presented in Table 9. The mean BCF_{SS} values (from day 21 to day 56) are 1,645 ± 361 L/kg (low concentration) and 1,807 ± 361 L/kg (high concentration). Lipid content (4.3% at study initiation) was assumed to remain constant throughout the study as no increase in fish weight was observed. The lipid-normalised mean steady-state bioconcentration factor (BCF_{SSL}) was 1,912 ± 420 L/kg (low concentration) and 2,101 ± 420 L/kg (high concentration).

Table 9: Concentrations in water (µg/mL) and fish (µg/g), and BCF values for the bioaccumulation study (unpublished, 1999)

Day	Concentration			BCF_{SS} (L/kg)		$BCF_{SS,L}$ (L/kg)	
	Water (mg/L)	Fish (mg/kg)					
		A	B	A	B	A	B
Low concentration							
7	0.0177	8.51	6.99	481	395	559	459
14	0.0184	15.5	18.8	842	1,022	980	1,188
21	0.0189	25	32.8	1,323	1,735	1,538	2,018
28	0.0186	26.1	40.8	1,403	2,194	1,632	2,551
42	0.0183	34.2	22.2	1,869	1,213	2,173	1,411
56	0.0181	36.6	25.3	2,022	1,398	2,351	1,625
High concentration							
7	0.183	54.9	60	300	328	349	381
14	0.181	157	116	867	641	1,009	745
21	0.179	235	386	1,313	2,156	1,527	2,507
28	0.179	228	310	1,274	1,732	1,481	2,014
42	0.179	442	449	2,469	2,508	2,871	2,917
56	0.178	297	238	1,669	1,337	1,940	1,555

Concentrations of TPPT after 1 week of depuration were 0.271 and 0.0734 mg/kg ww in the low and high exposure concentrations, respectively. These values equated to 0.8 and 0.2% of the assumed steady-state concentrations at 56 days. ECHA (2024b) describes the depuration as remarkably high and not consistent with the relatively slow equilibrium in the uptake phase. Although the depuration rate is high, the Agency concludes that there is no strong evidence available to suggest that values reported for the extent of depuration are not reliable.

ECHA (2024b) presents BCF_k values based on the uptake phase only. The lipid-normalised values of 2,112 and 2,476 L/kg for the low and high exposure concentrations were verified by the Agency after independent plotting and fitting of the reported study data. The Agency repeated the exercise to include the depuration data using the simultaneous method for calculation of uptake and depuration rate constants. This resulted in lipid-normalised BCF_k values of 1,740 L/kg for the low exposure concentration and 1,985 L/kg for the high exposure concentration. The Agency notes that these values are uncertain because only one datapoint (in replicate) was available for the

depuration and specifically for the low concentration, the measurement was close to the limit of detection of the analytical method, and it is not possible to determine with confidence where this data point would fall on the depuration curve.

ECHA (2024b) discusses the likely suppression of TPPT solubility due to the presence of more hydrophobic components and uses two methods based on Raoult's Law to re-calculate the dissolved concentrations of TPPT to 0.0132 and 0.0136 mg/L for the nominal test substance concentration of 0.05 mg/L; this corresponded to 75 and 77% of the TPPT of the concentration measured in the dilution water. ECHA (2024b) concludes the BCF values should be substantially higher and could be close to the vB criterion. The Agency recognises that dissolved concentrations of TPPT may be lower than used in the BCF calculations but that there is no clear evidence to support this assertion. The calculations using Raoult's Law have not been checked by the Agency as they were not presented in sufficient detail.

The Agency concludes that the study can be assigned Klimisch score 2 but that only the results from exposure of fish to 0.05 mg/L of test substance are considered reliable.

2.3.2.1.4 Bioaccumulation in terrestrial organisms (soil dwelling organisms, vertebrates)

The log of the predicted octanol-air partition coefficient (log K_{OA}) for TPPT is 10.09 (using KOAWIN v1.10 of EPISuite™). It was concluded that TPPT was within the applicability domain of the model because the estimated value relies on the estimated K_{OW} and Henry's Law constants where it has already been concluded that TPPT was within the applicability domain by ECHA (2024b). Log K_{OW} for TPPT is > 2 and the estimated log K_{OA} is > 5, therefore TPPT screens as bioaccumulative in air-breathing organisms.

2.3.2.2 Summary and discussion of bioaccumulation

TPPT screens as potentially B/vB in aquatic organisms and air breathing organisms based on physicochemical data. Estimated BCF values using the BET assessment within EAS-E-Suite were 2,320 and 2,340 L/kg based on dissolved or total substance in the aqueous phase, respectively.

The Agency notes that the low water solubility and high log K_{OW} value indicate that dietary exposure would have been appropriate for the definitive fish bioaccumulation study with TPPT, but that OECD TG 305 did not include an option for a dietary study until the 2012 revision. The only available *in vivo* fish bioaccumulation study used aqueous exposure enhanced with a solubiliser and reports a mean lipid normalised BCF_{SSL} value for the low concentration of 1,912 ± 420 L/kg; only two fish were sampled at each time point, but four out of eight individual BCF values measured during the steady-state phase were above 2,000 L/kg. The BCF_{SSL} value from the high exposure concentration was 2,101 ± 420 L/kg but the Agency considers that this data should not be used in the bioaccumulation

assessment given that two validity criteria were failed. The lipid normalised BCF_k values were 2,112 and 2,476 L/kg for the low and high exposure concentrations when based solely on uptake data and were 1,740 L/kg for the and 1,985 L/kg, respectively, when depuration data were included (although this introduces significant uncertainty). Again, the Agency opinion is that the data from the high exposure concentration should not be used in the bioaccumulation assessment. Overall, the Agency concludes from the evidence available and considered reliable that TPPT has the potential to bioaccumulate in the aquatic environment.

2.4 Environmental hazard assessment

2.4.1 Aquatic compartment (including sediment)

2.4.1.1 Fish

2.4.1.1.1 Short-term toxicity to fish

ECHA (2024b) concluded that no reliable acute fish studies were available. All identified studies, including those of limited reliability, are summarised in Table 10.

Table 10: Summary of acute fish toxicity studies presented in ECHA (2024b)

Reference	Study details	Results
Unpublished study (2002)	OECD TG 203 *Danio rerio* (Zebrafish) TPPT (0.45 µm filtered 100 mg/L solution) Duration: 96 hours Klimisch score 3	There was no analysis of test substance concentrations. There was undissolved material in the test vessels after 24 hours. No toxic effects observed.
Unpublished study (2002)	OECD TG 203 *Danio rerio* (Zebrafish) exposed to TPPT (Eight concentrations from 1.8 to 100 mg/L; prepared using dispersant/solvent). Duration: 96 hours Klimisch score 3	The three highest concentrations (range 32 to 100 mg/L) had undissolved test material visible after 24 hours and were the concentrations where mortality occurred. Observed LC_{50} was 83 mg/L.

2.4.1.1.2 Long-term toxicity to fish

ECHA (2024b) identified two reliable chronic fish toxicity studies: one conducted with TPPT as the test substance, and another using a reaction mass of triphenylthiophosphate and tert-butylated derivatives (EC no. 421-820-9). Studies are summarised in Table 11.

Table 11: Summary of chronic fish toxicity studies presented in ECHA (2024b)

Reference	Study details	Results
Unpublished study (2023)	OECD TG 210 *Oncorhynchus mykiss* (Rainbow trout) exposed to TPPT Duration: 97 days (60 days post hatch) Klimisch score 1	97-d EC_{10} values: 2.1 µg/L (larval survival) and 2.2 µg/L (overall survival). 97-d EC_{50} values: 3.5 µg/L (larval survival) and 3.5 µg/L (overall survival). 97-d NOEC: 1.7 µg/L (post hatch survival).
Unpublished study (2003)	OECD TG 210 *Oncorhynchus mykiss* (Rainbow trout) exposed to reaction mass of triphenylthiophosphate and tert-butylated derivatives (EC no. 421-820-9). Duration: 87 days Klimisch score 2	Test substance: 87-d NOEC: 4.4 µg/L (growth rate) 87-d NOEC: 8.7 µg/L (survival after thinning) 87-d NOEC: 8.7 µg/L (time to swim up) TPPT (calculated): 87-d EC_{10} values: 6.0 µg/L (percentage swim up) and 5.2 µg/L (larval survival after thinning). 87-d EC_{50} values: 6.4 µg/L (percentage swim up) and 6.7 µg/L (larval survival after thinning).

- Unpublished report (2023)

A flow-through early life stage study was conducted to OECD TG 210 and GLP with *Oncorhynchus mykiss* (Rainbow trout). The test substance was TPPT with aqueous solutions prepared by saturator columns. The time weighted average concentrations were reported as 0.26, 0.67, 1.7, 4.3, and 12 µg/L. There were 40 embryos per replicate (2 hours old at initiation), which were thinned to 20 on day 22 of incubation. Larvae of the 20 embryos were transferred to aquaria on day 37. Larvae were fed live brown shrimp nauplii from day 46. The test temperature was 9.5 to 11°C and the test duration was 97 days.

There were no significant effects on hatching success (85 to 91%) nor on live larvae (99-100%). Mean time to hatch was 31 days and to swim was 47 days. Post-hatch survival appeared to be the most sensitive endpoint; survival was as follows: control 100%, 98% at 0.26 µg/L, 98% at 0.67 µg/L, 95% at 1.7 µg/L, 27% at 4.3 µg/L, and 0% at 12 µg/L. The no-observed effect concentration (NOEC) for this endpoint was therefore 1.7 µg/L and the lowest observed effect concentration (LOEC) was 4.3 µg/L. Where mortality was low (up to 1.7 µg/L), length and weight of larvae were not significantly different from the controls.

All of the validity criteria stated in the guideline were met as summarised below and therefore the Agency agrees that this study can be considered reliable:

- Dissolved oxygen was > 60% of air saturation. The range reported in the EU REACH registration dossier was 71.4 to 99.9% saturation.

- The water temperature did not differ by more than ± 1.5°C (range was 9.5 to 11.0°C).
- Analytical measurement of the test concentration was carried out.
- The overall survival in the controls should be > 75% (hatching success and post-hatch success). Post-hatch survival was reported in the EU REACH registration dossier as 100%.

ECHA (2024b) reports that the study states that dose-response modelling is not possible, perhaps due to the steepness of the dose-response relationship. A log-logistic dose-response was fitted for larval survival (not shown) and for overall survival (plotted). The derived EC_{10} and EC_{50} values were 2.1 and 3.5 µg/L (larval survival) and 2.2 and 3.5 µg/L (overall survival). There was insufficient data available to check how these values were produced but the Agency agrees that they were in accordance with the reported NOEC (1.7 µg/L) and LOEC (4.3 µg/L).

- Unpublished report (2003)

A flow-through early life stage study was conducted to OECD TG 210 and to GLP with *Oncorhynchus mykiss* (Rainbow trout). The test substance was the reaction mass of triphenylthiophosphate and tert-butylated derivatives (EC no. 421-820-9); nominal test substance concentrations were 6.3, 13, 25, 50, and 100 µg/L; mean measured concentrations were 4.4, 8.7, 17, 29, and 66 µg/L based on measurement by GC-FPD. Two constituents that form the basis of the analysis are assumed in ECHA (2024b) to be TPPT and one of the mono-substituted tert-butyl derivatives of TPPT. The Agency has no means to check what was measured but notes that the method of analysis is non-specific. The test temperature was 11 to 13°C (slightly above that recommended in the guidance), dissolved oxygen content was 6.5 to 9.8 µg/L (the Agency assumes this is a transcription error and should be mg/L). Hatching success in the negative and solvent controls averaged 81 and 80%, respectively. Although the validity criteria were met, it was noted that not all of the test substance was dissolved, resulting in a slight oily film in the diluter mixing chambers that increased with concentration. ECHA (2024b) designated the study as Klimisch score 2. The Agency agrees based on the evidence available, although notes that it is not clear what exactly was measured analytically in this study.

Hatching success (78-86%) and time to hatch (23 to 27 days) were not affected in the exposure groups. Time to swim was significantly affected at 17 µg/L and was not reached in the two highest treatment groups. Swim-up percentages (day 16 post-hatching) were: 91% for the control and solvent control groups, 94% at 4.4 µg/L, 92% at 8.7 µg/L and 30% at 17 µg/L. Larval survival from day 16 to day 60 post-hatching was 100% for the control and solvent control groups, 100% at 4.4 µg/L, 97% at 8.7 µg/L and 53% at 17 µg/L. The endpoints are based on mean measured concentrations. All larvae died by day 29 post-hatch at the two highest concentrations. ECHA (2024b) concluded that some effects on growth (length/weight) were observed, for which the NOEC lies below 10 µg/L.

There was no dose-response modelling in the report but ECHA (2024b) reported

acceptable log-logistic dose-response model fitting for percentage of larvae that reached swim up stage by 16 days post-hatch and percentage survival of larvae after thinning. The EC_{10} and EC_{50} were 15.4 and 16.6 µg/L (swim up) and 13.8 and 17.2 µg/L (larvae survival), respectively. Overall survival calculated by ECHA (2024b) was 79% for the control and solvent control, 75% at 4.4 µg/L, 82% at 8.7 µg/L, 43% at 17 µg/L, 0% at both 29 µg/L and 66 µg/L.

TPPT is a significant constituent of the test substance, and the reported mean measured concentrations are equivalent to 1.3, 2.6, 5.2, 8.8, and 20 µg/L of TPPT based on its content in the test substance. This assumes that all constituents are equally soluble but the support document notes that more hydrophobic components than TPPT are present in the test substance. There was evidence that the test substance was not fully dissolved, and so Raoult's Law was used in ECHA (2024b) to calculate dissolved concentrations of TPPT from the nominal concentration of the test substance. The Agency notes that it not clear whether the application of Raoult's Law is appropriate and that there is insufficient detail to check these calculations. The EC_{10} and EC_{50} values based on the calculated TPPT dissolved concentrations were 6.0 and 6.4 µg/L (percentage swim up) and 5.2 and 6.7 µg/L (larval survival after thinning) respectively.

ECHA (2024b) concludes that this study supports the conclusions of the OECD TG 210 study conducted with TPPT, the latter showing slightly lower effect concentrations for TPPT. The Agency notes that the test substance contained other constituents, and the contribution they make to the observed effects is unknown. The assumption that the toxicity is explained by TPPT concentrations alone is a worst case approach. The Agency agrees that the study provides supporting evidence to the conclusions of the OECD TG 210 study conducted with TPPT.

2.4.1.2 Aquatic invertebrates

2.4.1.2.1 Short-term toxicity to aquatic invertebrates

ECHA (2024b) reported three acute invertebrate studies (summarised in Table 12) but all were given a Klimisch score of 3 for deficiencies including the use of concentrations that exceeded the water solubility of TPPT, the presence of undissolved material, and a lack of quantitative analytical monitoring, The Agency agrees with the conclusion that in general the relevance of these tests is low.

Table 12: Summary of acute invertebrate toxicity studies presented in ECHA (2024b)

Reference	Study details	Results
Unpublished study (2002)	OECD TG 202; neonate *Daphnia magna* exposed to TPPT. No analysis of actual concentrations. Klimisch score 3	No toxic effects were seen.
Unpublished study (1988)	OECD TG 202; neonate *Daphnia magna* exposed to TPPT; undissolved material was observed in all test solutions after 24 hours Klimisch score 3	The reported EC_{50} was 49 mg/L.
Unpublished study (1996)	OECD TG 202; neonate *Daphnia magna* exposed to the reaction mass of triphenylthiophosphate and tert-butylated derivatives (EC no. 421-820). Semi-quantitative analysis but not for effects concentrations. Klimisch score 3	No toxic effects were seen.

2.4.1.2.2 Long-term toxicity to aquatic invertebrates

ECHA (2024b) identified two reliable with restrictions chronic invertebrate studies; one with TPPT as the test substance and the other with the reaction mass of triphenyl thiophosphate and tert-butylated derivatives (EC no. 421-820-9) as the test substance. A further study was considered unreliable (Klimisch score 3). Studies are summarised in Table 13.

Table 13: Summary of chronic invertebrate toxicity studies presented in ECHA (2024b)

Reference	Study details	Results
Unpublished study (2021)	21-d static renewal OECD TG 211 test *Daphnia magna* (< 24 hours old). TPPT (saturated solution) Klimisch score 2	No effects observed. 21-d NOEC ≥ 7.24 µg/L (time weighted average mean measured concentration).
Unpublished study (2015)	22-d static renewal OECD TG 211 test *Daphnia magna.* Reaction mass of triphenylthiophosphate and tert-butylated derivatives (EC no. 421-820-9) at 5.5 mg/L (nominal). Klimisch score 3	No toxic effects recorded. 22-d NOEC for reproduction > 5.5 mg/L (based on nominal test concentration)
Unpublished study (2003)	21-d flow-through OECD TG 211 test *Daphnia magna*. Reaction mass of triphenylthiophosphate and tert-butylated derivatives (EC no. 421-820-9) between 4.9 and 150 µg/L (mean measured concentrations) Klimisch score 2	21-d NOEC of 7.9 to 9.7 µg/L (based on TPPT)

- Unpublished study (2021)

The Agency notes that this study with TPPT was conducted as a limit test. The validity criteria were met as there was no parent mortality and there was an average of 126 ± 20 offspring for each parent in the exposed group and 124 ± 16 in the controls. The study was rated Klimisch score 2 and the Agency has no reason to disagree with this designation. A 21-d NOEC ≥ 7.24 µg/L was reported, based on time weighted average (twa) mean measured concentrations in the test solutions. However, ECHA (2024b) notes that the test report states that there were low measured concentration values in the biotic samples before renewal. ECHA (2024b) has therefore presented a NOEC ≥ 3.9 µg/L based on twa mean measured concentrations for the biotic samples. The Agency has no access to the test report and so cannot check this value.

- Unpublished study (2015)

The unpublished study (2015) with the reaction mass of triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC no. 421-820-9) was considered unreliable (Klimisch score 3) in ECHA (2024b) based on variability in concentrations measured and no specific measurement of TPPT. The Agency agrees with this conclusion.

- Unpublished study (2003)

The validity criteria were stated to have been met in a second study with the reaction mass of triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC no. 421-820-9). Parent survival at the end of the test in the control, solvent control and mean measured concentrations of test substance of 4.9, 11, 26, 46 and 150 µg/L was 90, 85, 75, 95, 85, 65 and 65%, respectively. Analytical monitoring was carried out by GC-FPD and was based on the analysis of two constituents, one of which was assumed to be TPPT. The Agency notes that no evidence is presented or discussed that confirms that one of the constituents is TPPT. The number of offspring produced per day averaged 6.43, 7.97, 8.38, 7.76, 8.57, 8.64 and 5.79, respectively. The study was rated Klimisch score 2 because there were substances other than TPPT present and it was not possible to fully assign toxicity to TPPT. The Agency has no reason to disagree with this score. The most sensitive endpoint was for mortality with a 21-d NOEC of 26 µg/L (corresponding to 7.9 µg TPPT/L based on its proportion in the test substance, assuming equal solubility of all constituents). ECHA (2024b) presented refined NOEC values based on calculated dissolved TPPT concentrations determined using Raoult's Law. There was insufficient evidence presented for the Agency to consider or verify these values.

2.4.1.3 Algae and aquatic plants

2.4.1.3.1 Toxicity to algae and aquatic plants

Two algal studies were available but ECHA (2024b) considered them to be unreliable as exposure concentrations were not measured (summarised in Table 14). The Agency did not consider these studies in any detail.

Table 14: Summary of acute invertebrate toxicity studies presented in ECHA (2024b)

Reference	Study details	Results
Unpublished study (2013)	72-h OECD TG 201 test *Desmodesmus subspicatus* TPPT (100 mg/L solution filtered as a limit test) Exposure concentration unknown Klimisch score 3	No toxic effects observed
Unpublished study (1997)	72-h OECD TG *Desmodesmus subspicatus* *R*eaction mass of triphenylthiophosphate and tert-butylated derivatives (EC no. 421-820-9) (exposure concentration of TPPT unknown) Klimisch score 3	No toxic effects observed

2.4.2 Summary and discussion of environmental toxicity

The most sensitive chronic endpoints are a 97-d EC_{10} of 2.1 µg/L (larval survival) and 2.2 µg/L (overall survival), and a 97-d NOEC of 1.7 µg/L (post hatch survival) in *Oncorhynchus mykiss* (Rainbow trout). TPPT is a significant constituent of the reaction mass of triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC no. 421-820-9), and toxicity was also reported in a chronic fish study for that substance, with a lowest EC_{10} of 13.8 µg/L (larval survival). ECHA (2024b) makes various assumptions to estimate an equivalent TPPT concentration, which suggests an EC_{10} of the same order of magnitude as the study with TPPT itself. However, there were issues with solubility and it is possible that other constituents contributed to the overall toxicity, so the Agency considers that this study provides limited supporting evidence.

No adverse chronic effects were reported in a limit test with invertebrates (*Daphnia magna*) using a saturated solution of TPPT, with a reported 21-d NOEC of ≥ 7.24 µg/L. ECHA (2024b) recalculated this as ≥ 3.9 µg/L based on the measured concentrations in the exposure solutions, but details are lacking so the Agency cannot check how this was done. In contrast, significant toxicity was reported in a second chronic *Daphnia* study with the reaction mass of triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC no. 421-820-9), with a 21-d NOEC of 26 µg/L. Although the MSC support document presented NOEC values in terms of estimated TPPT concentrations, the methodology is unclear and a clear conclusion for TPPT cannot be drawn as other constituents were present.

Two algal toxicity studies are available but are considered unreliable.

2.5 Conclusions on the SVHC properties

2.5.1 PBT and vPvB assessment

2.5.1.1 Persistence

TPPT did not fulfil the criteria for ready or inherent biodegradability and therefore screens as potentially P/vP. Although photodegradation in air is rapid (half-life of 4 hours), partitioning to air is predicted to be very low. The degradation DT_{50} from an aerobic mineralisation study in water conducted at 12 ± 2°C (Klimisch score 1) is much longer than the time of the study (61 days) and therefore much longer than the P and vP criteria of Annex 13 of UK REACH (half-lives of 40 days and 60 days respectively).

The Agency concludes from the evidence available that TPPT fulfils the P and vP criteria of Annex 13 of UK REACH.

2.5.1.2 Bioaccumulation

TPPT screens as potentially B/vB in aquatic organisms and air breathing organisms.

Estimated BCF values using the BET assessment within EAS-E-Suite were 2,320 and 2,340 L/kg based on dissolved or total substance in the aqueous phase respectively. The BCF_{SSL} value from a flow-through bioaccumulation study using Common carp (*Cyprinus carpio*) and a measured TPPT test concentration of 0.0183 mg/L was calculated at each timepoint in the uptake phase where steady state was assumed to be reached. The mean value was 1,912 ± 420 L/kg with four out of eight values above 2,000 L/kg. The lipid normalised BCF_k value was 2,112 L/kg when based solely on uptake data.

The Agency concludes that there is sufficient evidence to conclude that TPPT fulfils the B criterion of Annex 13 of UK REACH (BCF higher than 2,000 L/kg).

2.5.1.3 Toxicity

The most sensitive chronic ecotoxicity endpoint for TPPT was for *Oncorhynchus mykiss* (Rainbow trout) with 97-d EC_{10} values of 2.1 µg/L (larval survival) and 2.2 µg/L (overall survival) and 97-d NOEC of 1.7 µg/L (post hatch survival). The NOEC is less than the threshold criterion of 0.01 mg/L (10 µg/L) stated in Annex 13 of UK REACH and therefore the Agency concludes that TPPT fulfils the T criterion.

2.5.1.4 Overall conclusions on the PBT and vPvB properties

Based on the information available, the Agency concludes that TPPT fulfils the PBT criteria of Annex 13 of UK REACH and can therefore be identified as an SVHC in accordance with Article 57(d) of UK REACH.

3. Information on use, exposure and alternatives

3.1 UK and EU REACH registration status and tonnage

Under UK REACH, the substance is registered with an aggregated tonnage of 100-1000 tonnes per annum (tpa).

In addition, a total of 39 Downstream User Import Notifications (DUINs[2]) have been submitted.

Under EU REACH, the substance is registered with an aggregated tonnage of 100 to 1000 tpa.

3.2 General description of uses and exposure

TPPT is primarily used in enclosed industrial and professional applications, particularly as a component of lubricants and greases, in hydraulic fluids and metal working fluids (ECHA, 2024c).

Environmental release may occur during the formulation of mixtures containing TPPT and through use as a processing aid at industrial sites.

ECHA (2024c) also reports potential consumer uses of TPPT in lubricants and greases. However, these are generally associated with closed systems with low release potential, such as in cooling liquids in refrigerators and in hydraulic liquids in automotive suspension systems.

Overall, TPPT exhibits a predominantly industrial and professional use profile, with exposure largely confined to controlled operational settings.

3.3 Alternatives

A range of alternatives are reportedly available for TPPT when used as a lubricant additive (ECHA, 2024c). These include phosphorus-based additives (e.g. zinc dialkyldithiophosphates, tricresyl phosphate and phosphite esters), sulphur-based additives (e.g. sulphurised olefins and dithiocarbamates), boron-based additives (e.g. boron esters and boron nitride), organic additives (e.g. polyol esters and glycerol

[2] 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.

monooleate), and molybdenum-based additives (e.g. molybdenum disulphide and molybdenum dialkyldithiocarbamates).

At present, these alternatives have not been comprehensively assessed. There is insufficient information to determine whether they possess similar hazard profiles or whether they can be considered suitable substitutes.

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Glossary

Agency, the	HSE
B	Bioaccumulative
BAF	Bioaccumulation factor
BCF	Bioconcentration factor
CAS	Chemical Abstracts Service
DT_{50}	Time taken for 50% decline in mass or concentration. If the decline is described by first order kinetics then this is also called the half-life
DU	Downstream User
DUIN	Downstream User Import Notification
ECHA	European Chemicals Agency
EC	European Community
EC_{10}	Effective concentration at 10% effect
EC_{50}	Effective concentration at 50% effect
EU	European Union
HLB	Elimination half-life
IUPAC	International Union of Pure and Applied Chemistry
K_{OA}	n-Octanol-air partition coefficient
K_{OW}	n-Octanol–water partition coefficient
LOEC	Lowest observed effect concentration
MCL	Mandatory classification and labelling
MSC	EU Member State Committee
NOEC	No observed effect concentration
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
SVHC	Substance of very high concern
TG	Test guideline
TPA	Tonnes per annum
TPPT	O,O,O-triphenyl phosphorothioate
vB	Very bioaccumulative
vP	Very persistent
vPvB	Very persistent and very bioaccumulative

Appendix A: Estimated and predicted data – Eas-E Suite™ [3]

The Agency followed the following steps to generate estimation data for bioaccumulation endpoints of O,O,O-triphenyl phosphothioate (TPPT)

- TPPT was located in EAS-S Suite through the CAS number (597-82-0).
- Input data were refined before initialisation of the Bioaccumulation Estimation Tool (BET):
    1. User input of the mean of the experimentally measured values provided in the registration dossier for the octanol water partition coefficient - log K_{OW} 4.9 (Table S1). The original consensus estimation was > 5.5
    2. The consensus value of QSARIN and IFQSAR estimations for whole body fish-half (HLB) (Table S2)
    3. The HLB value from IFQSAR estimation
    4. The upper and lower HLB value from QSARIN estimations
    5. More detailed input parameters for the BET estimations are detailed in Table S3
- IFSQSAR Version 1.1.2 (Table S4) and QSARIN-Chem estimations and predictions were made for selected parameters
- The QMRF for the Arnot-Gobas BCFBAF model is available for download from Documents - ARC Arnot Research & Consulting)
- Only one Only one of the 572 chemicals with measured laboratory BCF data used to evaluate the Arnot-Gobas BCFBAF model for the QMRF is a thiophosphate

[3] EAS-E Suite (Ver.0.982 - BETA, release January 2026). www.eas-e-suite.com. Accessed 17th April 2026. Developed by ARC Arnot Research and Consulting Inc., Toronto, ON, Canada

Table A1: BET - 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 (inc. consensus HLB)	297	0.121	2,430	2,450
Generic Lab Fish (no HLB)	297	0.0057	5,160	5,210

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.

Table A2: BET - 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)	BMFA* Growth Cor. (gut temperature) (activity/activity; Ingesta)
Generic Lab Fish	0.00759	0.00	0.121	0.188	0.217	0.217	0.191	0.221	0.221
Generic Lab Rat	0.054	0.114	4.47e+00	0.0067	0.00646	0.00646	0.0067	0.00646	0.00646

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.

Table A3: IFSQSAR Version 1.1.2

Model	endpoint	units	qsarpred	UL	AD	error
logKow	Log of wet (practical) octanol-water partition coefficient (log P) - updated for PFAS	log L[w]/L[wet o]	6.27	2	in	1.19
logKoa	Log of octanol-air partition coefficient - updated for PFAS	log L[a]/L[o]	11.67	2	in	0.94
fhlb	Whole body biotransformation half-life in reference fish (0.01kg, 15degC)	hours	83.34	1	in	30.78
hhlb	Whole body biotransformation half-life in reference human (70kg)	hours	20.95	0	in	20.64

Table A4: QSARINS-Chem Model

Model	pred	unit	hat	desc_range	high_leverage	pred_range	AD
FishM1	332.66	Hour	0.012723	OK	No	In	OK
FishM2	81.096	Hour	0.011429	OK	No	In	OK
FishM3	191.426	Hour	0.013852	OK	No	In	OK

Table S1: Initialised chemical input parameters - Bioaccumulation Estimation Tool (BET)

Symbol	Parameter	Unit	Value	Notes
Name	Chemical name	O,O,O-triphenyl phosphorothioate		
CAS	Chemical abstract service registration number	000597-82-0		
SMILES	SMILES notation	S=P(Oc1ccccc1)(Oc1ccccc1)Oc1ccccc1		
M	Molar mass	g/mol	342.35	
Log KOW,N	log10 octanol-water partition ratio, neutral	L/L	4.9	Manual input – Experimental data from OECD TG 117 studies (Consensus of 4.79 + 5.0)
Log KOA,N	log10 octanol-air partition ratio, neutral	L/L	11.165	
Log KSlW,N	log10 storage lipid-water partition ratio, neutral	L/L	6.45	
Log KMlW,N	log10 membrane lipid-water partition ratio, neutral	L/L	5.94	
Log KPrW,N	log10 protein-water partition ratio, neutral	L/L	4.56	
Log KSaW,N	log10 serum albumin-water partition ratio, neutral	L/L	5.01	
BP	Boiling point	Celsius	463.42	
MP	Melting point	Celsius	68.437	
VP	Vapor pressure	Pa	1.27E-05	
WatSol	Water solubility	mg/L	0.0288	
BioHL - fish	Biotransformation half-life fish (@ 0.01kg)	Hours	137.22	Refined to 144.04 - Table S2
BioHL - mammal	Biotransformation half-life mammal (@ 70kg)	Hours	15.24	

Symbol	Parameter	Unit	Value	Notes
EnvHL - outdoor air	Degradation half-life outdoor air	Hours	6.03	
EnvHL - surface water	Degradation half-life surface water	Hours	465.07	
EnvHL - sediment	Degradation half-life sediment/solid	Hours	4185.63	
EnvHL - indoor air	Degradation half-life indoor air	Hours	12.06	
EnvHL - soil	Degradation half-life soil	Hours	930.14	
Scaling Factor KPrW	Scaling Log KPrW, A	Unitless	1	
Scaling Factor KPrW	Scaling Log KPrW, B	Unitless	1	
IRT	Intake rate threshold	mg/kg-ww/d	0.0028	
IEC	Internal effect concentrationï¿½	mmol/kg-ww	5.00E-07	
iTTC	Internal Threshold of Toxicological Concern	nmol/L-Blood	0.1	

Table S2: Refinement of the BET chemical input parameters using IFQSAR and QSARINs

Symbol	Parameter	Unit	Value	Notes
BioHL - fish	Biotransformation half-life fish (@ 0.01kg)	Hours	144.04	Adjusted from 137.22 at default setting to use consensus prediction from: IFSQSAR fhlb-IFS; Prediction: 83.34; AD:OK; Note: NA QSARINS FishM1-Molecular descriptors; Prediction: 332.66; AD:OK; Note: NA QSARINS FishM2-Molecular descriptors; Prediction: 81.1; AD:OK; Note: NA QSARINS FishM3-Molecular descriptors; Prediction: 191.43; AD:OK; Note: NA

AD: Applicability domain

Table S3: Additional detailed BET input following refinements

Symbol	Parameter	Unit	Value
Log KCbW (neutral)	log10 carbon–biota (or carbon–biological phase) to water partition ratio	L/L	2.170425
Invertebrates HL	Half-life in invertebrates	h	432.12
Fish HL	Half-life in fish	h	144.04
Mammal HL	Half-life in mammal	h	15.24
Avian HL	Half-life in avian	h	15.80635
Lab Rat HL	Half-life in rat	h	3.725593
Plant HL	Half-life plant	h	1×10^{12}

Supplementary Information IFSQSAR Version 1.1.2

IFSQSARs use a group contribution model, in which specific substructures of a molecule are counted, and their contributions are determined by multiple linear regression. All IFSQSARs have a defined applicability domain (AD) and estimates of prediction uncertainty. For most models the prediction uncertainty is in the form of an estimated standard error of prediction. For the models which predict half-lives the standard errors of prediction have been converted from log-scale to factor errors, also called dispersion or confidence factors. The AD in IFSQSARs uses - chemical similarity, leverage, functional group checks, and boundary conditions. Models output an uncertainty level (UL) which flags if the prediction violates different AD checks. Interpretation of UL can vary between models, so IFSQSAR gives an overall assessment of in or out of AD.

UL	AD	Description
0	in	no AD warnings
1	in	similarity or leverage indicate prediction close to edge of training data
2	in or out	similarity or leverage indicate extrapolation, can be in AD if validated
3	out	leverage indicates extreme extrapolation
4	in or out	zero fragment counts, in AD if model intercept is meaningful
5	out	functional group not contained in training data
6	out	boundary condition exceeded

IFSQSAR outputs UL, AD, and other data with every prediction:

Output	Description
Input SMILES	SMILES entered by user
Canonical SMILES	SMILES after applying internal normalization
SMILES Note	Description of any modifications by the SMILES normalizer
Model	Which model was applied
endpoint	Description of the endpoint the model predicts
units	Units of the predicted value
qsarpred	The value predicted by the model
UL	Uncertainty Level as described above
AD	Applicability Domain, in or out
error	Prediction uncertainty as described above
ULnote	More descriptive UL and AD warnings
citation	Literature citation for paper that describes the model

Table S4: IFQSAR outputs for TPPT

Model	endpoint	units	qsarpred	UL	AD	error	ULnote
logKow	Log of wet (practical) octanol-water partition coefficient (log P) - updated for PFAS	log L[w]/L[wet o]	6.27	2	in	1.19	solute 1 dependency ULs: S=1, A=4, B=2, Vf=na, L=2, aggregate UL is out of the AD because a dependency is out of the AD, classified as in AD because of uncertainty validation
logKoa	Log of octanol-air partition coefficient - updated for PFAS	log L[a]/L[o]	11.67	2	in	0.94	solute 1 dependency ULs: S=1, A=4, B=2, Vf=, L=2, aggregate UL is out of the AD because a dependency is out of the AD, classified as in AD because of uncertainty validation
logKoc	Log of organic carbon-water partition coefficient (log Koc by Bronner *et al.*)	log L[w]/kg[OC]	5.09	2	out	1.22	solute 1 dependency ULs: S=1, A=4, B=2, V=, L=2, aggregate UL is out of the AD because a dependency is out of the AD
logVPliquid	Log of vapor pressure of liquid or super-cooled liquid predicted by PPLFER at 298K - updated for PFAS	log Pa	-5.1	2	in	2.2	solute 1 dependency ULs: S=1, A=4, B=2, Vf=, L=2, state=3, MVliquid=na; aggregate UL is out of the AD because a dependency is out of the AD; classified as in AD because of uncertainty validation
logSwliquid	Log of solubility for liquids or super-cooled liquid solutes in water predicted by PPLFER at 298K - updated for PFAS	log mol/L[w]	-6.07	2	in	1.78	solute 1 dependency ULs: S=1, A=4, B=2, Vf=, L=2, state=3, MVliquid=; aggregate UL is out of the AD because a dependency is out of the AD; classified as in AD because of uncertainty validation
logVP	Log of vapor pressure at 298K	log Pa	-5.79	3	out	2.2	solute 1 dependency ULs: S=1, A=4, B=2, Vf=, L=2, state=3, MVliquid=, MVsolid=, tmconsensus=3, tm=3, dsm=2; aggregate UL is out of the AD because a dependency is out of the AD; liquid state PPLFER adjusted for solid solute
logSw	Log of solubility in water at 298K	log mol/L[w]	-6.75	3	out	1.78	solute 1 dependency ULs: S=1, A=4, B=2, Vf=, L=2, state=3, MVliquid=, MVsolid=, tmconsensus=3, tm=3, dsm=2; aggregate UL

Model	endpoint	units	qsarpred	UL	AD	error	ULnote
							is out of the AD because a dependency is out of the AD; liquid state PPLFER adjusted for solid solute
logSoliquid	Log of solubility in dry octanol for liquid or super-cooled liquid solute - updated for PFAS	log mol/L	0.17	2	in	1.08	solute 1 dependency ULs: S=1, A=4, B=2, Vf=, L=2, state=3, MVliquid=; aggregate UL is out of the AD because a dependency is out of the AD; classified as in AD because of uncertainty validation
dsm	Entropy of fusion	J/mol.K	94.64	2	out	22.61	structural outlier
fhlb	Whole body biotransformation half-life in reference fish (0.01kg, 15degC)	hours	83.34	1	in	30.78	high leverage
hhlb	Whole body biotransformation half-life in reference human (70kg)	hours	20.95	0	in	20.64	
hhlt	Whole body total elimination (terminal) half-life in reference human (70kg)	hours	3.4	2	out	56.1	out of domain
HLbiodeg	Biodegradation half-life in water (20-25degC)	hours	328.25			149.83	generic error estimated from uncertainties of model fits
koh	kOH - rate constant of reaction with hydroxyl radicals in air at 298K	cm^3/molec.s	2.75E-09	1	in	13.70251	high leverage
ko3	kO3 - rate constant of reaction with ozone in air at 298K	cm^3/molec.s	3.47E-17	5	out	506.7573	leverage > 1, Sulphur atom with bond count not in training set, Sulphur atom with total bond order (valence) not in training set
E	Abraham PPLFER solute descriptor E - excess molar refractivity - updated for PFAS		2.279	2	out	0.178	out of domain
S	Abraham PPLFER solute descriptor S - dipolarity/polarizability - updated for PFAS		1.9	1	in	0.3	low similarity
A	Abraham PPLFER solute descriptor A - hydrogen bond acidity - updated for PFAS		0	4	in	0.032	no fragment overlaps with training dataset
B	Abraham PPLFER solute descriptor B - hydrogen bond basicity - updated for PFAS		0.64	2	out	0.23	out of domain
L	Abraham PPLFER solute descriptor L - log of hexadecane/air partition coefficient - updated for PFAS		11.32	2	out	0.74	out of domain
V	Abraham PPLFER solute descriptor V - McGowan Volume	0.01 cm^3/mol	2.476				
s	Abraham/Goss PPLFER system parameter s for solvent-air partitioning as log Ksa	unitless	4.685	2	out	0.396	out of domain, structural outlier
a	Abraham/Goss PPLFER system parameter a for solvent-air partitioning as log Ksa	unitless	5.511	2	out	0.937	structural outlier

Model	endpoint	units	qsarpred	UL	AD	error	ULnote
b	Abraham/Goss PPLFER system parameter b for solvent-air partitioning as log Ksa	unitless	0	4	in	0.08	no fragment overlaps with training dataset
v	Abraham/Goss PPLFER system parameter v for solvent-air partitioning as log Ksa	unitless	-0.823	2	out	0.195	structural outlier
l	Abraham/Goss PPLFER system parameter l for solvent-air partitioning as log Ksa	unitless	1.075	2	out	0.047	structural outlier
c	Abraham/Goss PPLFER system parameter c for solvent-air partitioning as log Ksa	unitless	-0.65	2	out	0.077	structural outlier

Further information

This publication is available on the HSE website here.

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