Substance Name: O,O,O-triphenyl phosphorothioate

EC Number: 209-909-9

CAS Number: 597-82-0

Substance Name:

Reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives

EC Number: 421-820-9

CAS Number: 192268-65-8

MEMBER STATE COMMITTEE SUPPORT DOCUMENT FOR IDENTIFICATION OF

O,O,O-TRIPHENYL PHOSPHOROTHIOATE AND

REACTION MASS OF: TRIPHENYLTHIOPHOSPHATE AND TERTIARY BUTYLATED PHENYL DERIVATIVES

AS SUBSTANCES OF VERY HIGH CONCERN BECAUSE OF THEIR PBT (ARTICLE 57D) PROPERTIES

Adopted on 22 November 2024

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TABLES

ABBREVIATIONS

B: Bioaccumulative
BCF: Bio Concentration Factor
BCF_K: Kinetic bioconcentration factor
BCF_{KL}: Lipid normalised kinetic bioconcentration factor
BCF_{SS}: Steady-state bioconcentration factor
CLP: Classification, labelling and packaging (of substances and mixtures)
DMF: Dimethyl formamide
DOC: Dissolved Organic Carbon
DT50: Degradation half-life Time
dw: dry weight
EC: European Community
EU: European Union
EC10: 10% Effect Concentration
EC50: 50% Effect Concentration
ECHA: European Chemicals Agency
FID: Flame ionisation detector
FPD: Flame photometric detector
GC: Gas chromatography
GLP: Good Laboratory Practice
HPLC: High Performance Liquid Chromatography
IUPAC: International Union of Pure and Applied Chemistry
k_1: Uptake rate constant
k_2: Depuration rate constant
K_{oa}: Octanol-air partition coefficient
K_{oc}: Organic carbon normalised adsorption coefficient
K_{ow}: Octanol-water partition coefficient
LOEC: Lowest Observed Effect Concentration
LOQ: Limit of quantification
LRTP: Long Range Transport Potential
MS: Mass spectrometry
MS/MS: Tandem mass spectrometry
NOEC: No observed effect concentration
OECD: Organisation for Economic Cooperation and Development
PBT: Persistent, Bioaccumulative and Toxic

QSAR: Quantitative Structure-Activity Relationship
RAM: Radioactivity detector
REACH: Registration, Evaluation, Authorisation and Restriction of Chemicals
SVHC: substance of very high concern
TG: Test Guideline
TOC: Total Organic Carbon
TPPT: Triphenylphosphorothioate
TPP: Triphenylphosphate
vPvB: very Persistent and very Bioaccumulative

IDENTIFICATION OF SUBSTANCES OF VERY HIGH CONCERN ON THE BASIS OF THE CRITERIA SET OUT IN REACH ARTICLE 57

Substance name: O,O,O-triphenyl phosphorothioate (TPPT)

EC number: 209-909-9

CAS number: 597-82-0

And

Substance name: Reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives

EC number: 421-820-9

CAS number: 192268-65-8

- The substances are identified as persistent, bioaccumulative and toxic (PBT) according to Article 57 (d) of Regulation (EC) No 1907/2006 (REACH).

Summary of how the substances meet the criteria set out in Article 57 of the REACH Regulation

A weight-of-evidence determination according to the provisions of Annex XIII of REACH is used to identify the substance O,O,O-triphenyl phosphorothioate (TPPT) as a PBT substance. All available information (such as the results of standard tests and modelling, analogue approach (read-across) and (Q)SAR results) was considered together in a weight-of-evidence approach. As reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives contains more than 0.1% TPPT, this substance can also be identified as a PBT substance.

Persistence

QSARs predictions on biodegradation indicate borderline persistence. Reliable screening tests of ready biodegradability according to OECD TG 301B, C and D with either TPPT or Reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9) show that TPPT is not readily biodegradable with mineralisation generally below 20% after 28 days. The ready biodegradability studies are given a medium weight in the weight of evidence assessment.

In a reliable simulation test with natural pond water, performed on TPPT according to OECD TG 309, there was no indication of any significant degradation over the test duration of 61 days, while the reference substance showed high mineralisation in 14 days. It can thus be concluded that the half-life in fresh surface water is >>61 days. The simulation test is given a high weight in the weight of evidence assessment.

Further, a hydrolysis test according to OECD TG 111 performed on TPPT showed that primary degradation by abiotic hydrolysis is slow with an extrapolated aqueous half-life of 278 days at pH 7 and 12 °C.

The outcome of the simulation test in water together with the results of the screening tests and the hydrolysis test, leads to the conclusion that TPPT meets the 'persistence' criterion (P) and the 'very persistent' criterion (vP) in accordance with Annex XIII, points 1.1.1 and 1.2.1, of the REACH Regulation on the basis of its persistent and very persistent (P/vP) properties in fresh water (degradation half-lives > 60 days).

Bioaccumulation

The screening criteria for bioaccumulation in aquatic organisms (log $K_{ow} > 4.5$) is fulfilled for TPPT based on the measured log K_{ow} value of 5.0 estimated by the HPLC method (OECD TG 117).

A bioaccumulation study performed with carp exposed to Reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9) shows bioconcentration factors for TPPT close to or exceeding 2000, based on the low exposure test concentration which is the reliable part of the study (Klimisch 2). Normalised to 5% lipids, kinetic BCF_{KL}s based on the data from the uptake phase are in excess of 2000 (2112 L/kg for the lower tested concentration). When accounting for the reduced bioavailability, due to the application of TPPT in a mixture, the BCF values for TPPT would turn out even higher. The study was conducted to GLP following the Japanese test guideline "Bioaccumulation test of a chemical substance in fish or shellfish" provided in "the Notice on the Test Method Concerning New Chemical Substances" and is considered to be reliable with restrictions. The fish bioaccumulation test is given a high weight in the weight of evidence assessment.

The outcome of the fish bioaccumulation test together with the fact that the measured log K_{ow} of TPPT is >4.5 leads to the conclusion that TPPT meets the 'bioaccumulative' criterion (B) in accordance with Annex XIII, point 1.1.2 of the REACH Regulation on the basis of its bioaccumulative properties in fish (fish BCF > 2000).

Toxicity

A fish early life stage test according to OECD TG 210 performed on TPPT with rainbow trout under flow-through conditions resulted in a larval survival NOEC for TPPT of 1.7 µg/L, which is below the toxicity criterion of 10 µg/L. This test is reliable and is given a high weight in the weight of evidence assessment.

A toxicity test with Reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9) was performed on rainbow trout according to OECD TG 210. Although the dose-response modelling is hampered by the steep-dose response, it is clear that the EC10s are between the concentrations of 8.7 and 17 µg/L. If the toxicity of the mixture would be fully attributed to TPPT, the EC10 for larval survival would be 4.2 µg/L, i.e. slightly higher than observed in the test with pure TPPT. This test is reliable with restrictions and is given a high weight in the weight of evidence assessment.

The results of the fish early life stage tests lead to the conclusion that TPPT meets the 'toxicity' criterion (T) in accordance with Annex XIII, point 1.1.3 of the REACH Regulation on the basis of its toxic properties to fish (fish NOEC < 10 µg/L).

Conclusion

TPPT is very persistent. In a simulation test in water according to OECD TG 309 there was no significant degradation of the substance over a period of 61 days, resulting in a half-life >>60 d and thus fulfilling the P and vP criteria.

TPPT is bioaccumulative. In a bioconcentration test with carp exposed to reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9), the kinetic BCF of TPPT normalised to 5% lipids exceeds the B criterion of 2000 L/kg, based on the low exposure test concentration which is the reliable part of the study (Klimisch 2).

TPPT is toxic. The NOEC for TPPT in a fish early life-stage test with rainbow trout was 1.7 µg/L for mortality, which is well below the T criterion of 10 µg/L.

In conclusion, TPPT can be identified as a PBT substance according to Art. 57(d) of REACH by comparing all relevant and available information listed in Annex XIII of REACH with the criteria set out in the same Annex, in a weight-of-evidence determination.

As reaction mass of: triphenylthiophosphate and tert-butylated phenyl derivatives (EC 421-820-9) contains more than 0.1% TPPT, this substance can also be identified as a PBT substance according to Art. 57(d) of REACH.

Registration dossiers submitted for O,O,O-triphenyl-phosphorothioate: Yes

Registration dossiers submitted for the reaction mass of: triphenylthiophosphate and its tert-butylated phenyl derivatives: Yes, inactive from February 2024 as the registrants ceased manufacture/import.

Justification

1. Identity of the substance and physical and chemical properties

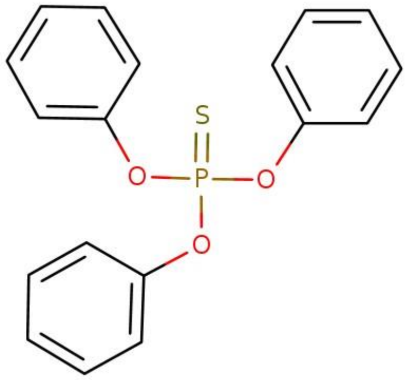
1.1 Name and other identifiers of the substance

The PBT assessment is focussed on O,O,O-triphenyl phosphorothioate (TPPT) that is registered as a mono-constituent substance. Based on this assessment, conclusions are also drawn for EC 421-820-9 'Reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives', containing more than 0.1% TPPT. EC 421-820-9 has also been used as test material for several relevant studies.

Table 1: Substance identity of TPPT

EC number:	209-909-9
EC name:	O,O,O-triphenyl phosphorothioate
CAS number (in the EC inventory):	597-82-0
CAS number:	597-82-0
IUPAC name:	O,O,O-triphenyl phosphorothioate
Index number in Annex VI of the CLP Regulation	
Molecular formula:	C18H15O3PS
Molecular weight range:	342.35
Synonyms:	Triphenyl phosphorothionate Triphenyl phosphorothioate O,O,O-Triphenyl thiophosphate Triphenyl thiophosphate Phosphorothioic acid, O,O,O-triphenyl ester Thiophosphoric acid triphenyl ester Triphenoxy(sulfanylidene)-lambda5-phosphane Phenyl phosphorothioate (PhO)3PS Aryl thiophosphate Tris(phenoxy)-sulfanylidenephosphorane

Structural formula:



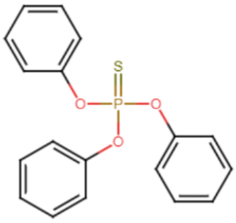
TPPT is also a constituent of the UVCB substance EC 421-820-9 'Reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives'. At present EC 421-820-9 has no active REACH registrations.

Table 2: Substance identity of Reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives

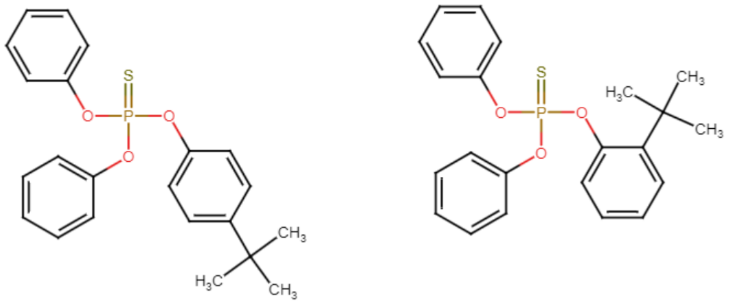
EC number:	421-820-9
EC name:	Reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives
CAS number (in the EC inventory):	192268-65-8
CAS number:	192268-65-8
IUPAC name:	-
Index number in Annex VI of the CLP Regulation	607-501-00-9
Index name in Annex VI of the CLP Regulation	Reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives
Molecular formula:	not applicable (UVCB)
Molecular weight range:	not applicable (UVCB)
Synonyms:	

Structural formula:

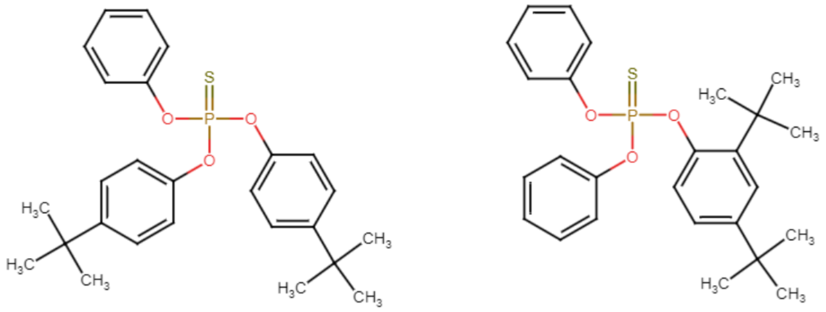
A non-exhaustive list of chemical structures that may be present in the composition of the substance is provided below:



O,O,O-triphenyl thiophosphate, EC 209-909-9



Examples of mono-*tert*-butyl O,O',O''-triphenylphosphorothioates



Examples of di-*tert*-butyl O,O',O''-triphenylphosphorothioates

1.2 Composition of the substance

Name: O,O,O-triphenyl phosphorothioate

Description: white crystalline, organic solid

Substance type: mono-constituent

Table 3: Constituents other than impurities/additives

Constituents	Typical concentration	Concentration range	Remarks
O,O,O-triphenyl phosphorothioate *EC 209-909-9*	≥ 80% (w/w)		

Also the following substance has been identified as relevant for the PBT assessment, as O,O,O-triphenyl phosphorothioate is a constituent.

Name: Reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives

Description: organic liquid. A combination of triphenylthiophosphate and *tert*-butylated triphenylthiophosphate constituents. Regarding the *tert*-butylated triphenylthiophosphates, the position and number of *tert*-butyl substituents on the phenyl rings is variable.

Substance type: UVCB

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

Not relevant for the SVHC assessment of the substance.

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

Not applicable

1.5 Physicochemical properties

The range of predicted solubilities of TPPT with QSARs is small and very close to the experimental value. Predicted log K_{ow} values from QSAR estimates are considerably higher than the values estimated by the HPLC method according to the OECD TG 117 (for both the single constituent and reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives). Only for the HPLC test with TTPT the reference compounds are given in the registration dossier. For this set, no substance with a phosphate group or a thiophosphate group were included and most substances were simple hydrocarbons.

The KOWWIN QSAR model identifies three substructure fragments contributing to the log K_{ow} estimation, which cover all the chemical functionality present in TPPT (aromatic carbon, thio-phosphorus and aromatic -O-P phosphate attachment). The training dataset of the KOWWIN model contains 40 substances with the thio-phosphorous group, with either one (like in TPPT) or two thio-phosphorous groups present. The validation dataset even contains 51 thio-phosphorous compounds. The -O-P aromatic phosphate ester attachment is present in 33 substances in the training dataset and in 68 substances in the validation dataset. Therefore organic (aromatic) thiophosphate esters are well represented in both training and validation datasets, and the prediction performance for the validation dataset can be taken as representative for the prediction performance for TPPT. Representative QSAR predicted log K_{ow} values are given for some organic aromatic thiophosphate esters which also have experimental reference values for log K_{ow}. These are given in Table 4, to illustrate the prediction precision (see column prediction error) for this type of substances for the USEPA KOWWIN QSAR model. Furthermore, for two of the aromatic phosphate-thio-esters the oxon (oxo-ester) version of the pesticide has a high quality log K_{ow} reference value (see Table 4). Both the predicted as well as the experimental log K_{ow} values for the oxon pesticide are 1.74-1.85 log units below the experimental and/or predicted log K_{ow} values of the thio-esters. If the same difference is applied extrapolating from the experimental (and predicted) log K_{ow} value for TPP, then values in the range of 6.33-6.55 would be expected for TPPT. This strengthens the assessment that the experimental (HPLC based) value for TPPT (5.0) should be considered as less reliable then the QSAR predictions, as the HPLC derived log K_{ow} value for TPPT is very close to the value for TPP (4.7), where a significant increase (1.74-1.85 log units) is expected based on the differences observed for aromatic oxon-phosphate and thio-phosphate esters.

Table 4 Examples of aromatic thiophosphate ester log K_{ow} QSAR predictions

Aromatic ring attached thiophosphate esters	**log K_{ow} QSAR (KOWWIN v1.68) prediction**	**Experimental log K_{ow} from PhysProp database**	**Physprop DB reference**	**Prediction error (log units)**
Diazinon	3.86	3.81	Hansch et al., 1995	0.05
Coumaphos	4.47	4.13	Tomlin, 1994	0.34
Chlorpyrifos	5.11	4.96	Sangster, 1994	0.15
Parathion	3.73	3.83	Hansch et al., 1995	0.10
Aromatic ring attached phosphate ester (not thio)				
Triphenyl phosphate	4.70	4.59	Hansch et al., 1995	0.11
Diazinon oxon	2.10	2.07	Hansch et al., 1995	0.03
Paraoxon	1.97	1.98	Sangster, 1994	0.01

One of the solubility estimation models (WSKOW v1.41) uses the log K_{ow} (estimated) as input, where the other water solubility model (WATERNT) relies on direct prediction from fragment model contributions. The (experimentally determined) low solubility is more in accordance with the high log K_{ow} values estimated by several QSARs and is not consistent with the low log K_{ow} values estimated by the HPLC method. The two water solubility estimation methods predict nearly identical values (0.021 versus 0.020 mg/L respectively), which are also in line with the experimentally determined value of 0.020 mg/L, supporting the conclusion that the QSAR estimates for octanol water partitioning (as well as for water solubility) are reliable and within the applicability domain and to be preferred over the approximation value determined by the HPLC method.

Table 5: Overview of physicochemical properties of TPPT

Property	**Description of key information**	**Value [Unit]**	**Reference/source of information**
Physical state at 20 °C and 101.3 kPa	solid crystalline, white		ECHA chemicals database for CAS 597-82-0[1]
Melting/freezing point	differential scanning calorimetry method according to OECD TG 113	ca. 53 °C at 101,325 Pa	ECHA chemicals database for CAS 597-82-0
	capillary method	53.2 °C	ECHA chemicals database for CAS 597-82-0
Boiling point	differential scanning calorimetry method according to OECD TG 113	Decomposes at >155 °C (1st reaction) and >255 °C (2nd reaction) without boiling at 101,325 Pa	ECHA chemicals database for CAS 597-82-0
	thermogravimetric analysis dynamic screening method	Decomposes at >225 °C	ECHA chemicals database for CAS 597-82-0

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[1] https://chem.echa.europa.eu/100.009.010/dossier-list/reach/dossiers/active?searchText=209-909-9

Property	Description of key information	Value [Unit]	Reference/source of information
Vapour pressure	effusion method, extrapolated values according to the OECD TG 104	0.0000136 Pa at 20 °C 0.0000301 Pa at 25 °C	ECHA chemicals database for CAS 597-82-0
	QSAR (Antoine method)	0.0000032 Pa at 25 °C	US EPA (2012), MPBPWIN v1.43
	QSAR (Modified Grain method)	0.000034 Pa at 25 °C	US EPA (2012), MPBPWIN v1.43
	QSAR (Mackay method)	0.0000683 Pa at 25 °C	US EPA (2012), MPBPWIN v1.43
	Subcooled liquid, QSAR (Antoine method)	0.000131 Pa at 25 °C	US EPA (2012), MPBPWIN v1.43
	QSAR, ACD/Labs software v11.02	0.0000383 Pa at 25 °C	ECHA chemicals database for CAS 597-82-0
Density	air comparison pycnometer (for solids)	1330 kg/m^3 at 25 °C	ECHA chemicals database for CAS 597-82-0
Water solubility	column elution method according to OECD test guideline 105	20 ± 3 µg/L at 20 °C and pH 7	ECHA chemicals database for CAS 597-82-0
	QSAR using log K_{ow} of 6.47	20.7 µg/L	US EPA (2012), WSKOW v1.41
	QSAR using fragment constants	19.6 µg/L	US EPA (2012), WATERNT
	QSAR	10^{-7} mol/L: ~34 µg/L	ChemAxon
Partition coefficient n-octanol/water (log value)	HPLC method according to OECD test guideline 117	log K_{ow} 5 at 23 °C and pH 6.4	ECHA chemicals database for CAS 597-82-0
	HPLC method according to OECD test guideline 117	log K_{ow} 4.79	ECHA chemicals database for CAS 192268-65-8[2]
	QSAR	5.45	ACD/Labs (2015) logP v14.03
	QSAR	5.98	ChemAxon, Consensus model
	QSAR	6.13	Biobyte (2006). Bio-Loom for Windows, v1.5
	QSAR	6.33	ChemAxon
	QSAR	6.47	US EPA (2012), KOWWIN v1.67

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[2] https://chem.echa.europa.eu/100.102.039/dossier-list/reach/dossiers/not_active?searchText=192268-65-8

Table 6: Overview of physicochemical properties of EC 421-820-9

Property	Description of key information	Value [Unit]	Reference/source of information
Physical state at 20°C and 101.3 kPa	Clear, yellowish liquid		ECHA chemicals database for CAS 192268-65-8
Melting/freezing point	Transition to glassy state, differential scanning calorimetry method according to OECD TG 102	-39 °C at 1013 hPa	ECHA chemicals database for CAS 192268-65-8
Boiling point	differential scanning calorimetry method (pinhole method) according to OECD TG 103	432 °C at 1013 hPa	ECHA chemicals database for CAS 192268-65-8
Vapour pressure	effusion method: vapour pressure balance according to OECD TG 104	0.00007 Pa at 20 °C 0.0001 Pa at 25 °C (extrapolated values)	ECHA chemicals database for CAS 192268-65-8
Density	Oscillating densitometer according to OECD TG 109	1167 kg/m^3 at 20 °C, 1151 kg/m^3 at 40 °C, 1153.7 kg/m^3 at 50 °C	ECHA chemicals database for CAS 192268-65-8
Water solubility	Flask method according to OECD TG 105	solubility of test substance < 0.1 mg/L at 20 °C at pH 6.2; solubility of main component TPPT ~ 0.1 mg/L, as shown by GC	ECHA chemicals database for CAS 192268-65-8
Partition coefficient n-octanol/water (log value)	HPLC method according to OECD test guideline 117	log K_{ow} 4.79 (main component) log K_{ow} 6.65 (o-*t*-butyl TPPT) log K_{ow} 6.97 (p-*t*-butyl TPPT)	ECHA chemicals database for CAS 192268-65-8

2. Harmonised classification and labelling

There is no current harmonised classification for TPPT.

Reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives is covered by Index number 607-501-00-9 in part 3 of Annex VI to the CLP Regulation as follows:

Table 7: Classification of EC 421-820-9 according to Annex VI, Table 3 (list of harmonised classification and labelling of hazardous substances) of Regulation (EC) No 1272/2008

Index No	Chemical name	EC No	CAS No	Classification		Labelling			Spec. Conc. Limits, M-factors and ATEs[3]	Notes
				Hazard Class and Category Code(s)	Hazard statement code(s)	Pictogram, Signal Word Code(s)	Hazard statement code(s)	Suppl. Hazard statement code(s)		
607-501-00-9	Reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives	421-820-9	192268-65-8	Aquatic Chronic 4	H413					

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[3] Acute Toxicity Estimate

3. Environmental fate properties

3.1 Degradation

3.1.1 Abiotic degradation

3.1.1.1 Hydrolysis

Hydrolysis was investigated at pH 4, 7, and 9 for TPPT at three temperatures up to 30 days according to OECD TG 111 (Unpublished study report, 2007). A concentration of 19 µg/L TPPT was tested. Hydrolysis was measured at 35 and 50 °C at pH 4 and 7 and at 20, 35 and 50 °C at pH 9. Analysis of parent compounds was done by HPLC-MS/MS. The following hydrolysis rates were obtained:

Table 8: Measured hydrolysis rates (k) of TPPT at different pH and temperature (Unpublished study report, 2007)

pH	Temperature [°C]	k [h^{-1}]
4	*35*	*0.00048*
4	*50*	*0.00116*
7	*35*	*0.0006*
7	*50*	*0.0015*
9	*20*	*0.0009*
9	*35*	*0.0020*
9	*50*	*0.0053*

Hydrolysis rates were not extrapolated to 12 °C, but from the presented data this can be calculated by means of the Arrhenius equation. The extrapolated half-lives for TPPT at 12 °C are 287, 278, and 60 days, at pH 4, 7, and 9 respectively (Klimisch score 2).

An earlier hydrolysis study was performed with reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives EC 421-820-9 (Unpublished study report, 1998). However, this was based on a loading of 3.4 g/L of the product, which is well above the water solubility of 20 µg/L. Hydrolysis was measured after filtration and indirectly by measurement of phenol formation. This test set-up was considered unsuitable for testing hydrolysis of TPPT due to the testing well in excess of the water solubility (Klimisch score 3).

Hydrowin v2.00 of US EPA EPI Suite (US EPA, 2012) only predicts a general (single) hydrolysis half-life for the group of phosphate esters as a whole. This estimate gives a minimum half-life of TPPT at pH 9 of 3.1 days and varies at other pHs between 9.2 and 10.5 days. The registration dossier of the analogue substance triphenyl phosphate, EC 204-112-2, has experimental data showing a much more rapid hydrolysis than TPPT[4]. Based on this, one series of values for the whole group of phosphate esters is not appropriate and the Hydrowin v2.00 prediction is considered to be not reliable.

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[4] https://chem.echa.europa.eu/100.003.739/dossier-view/9b2f054a-c82b-4cc1-9393-415a4f7781c1/IUC4-e6b5d811-aba2-31b0-b7d2-215f47e23be4_8c1aeebd-fd78-4661-8347-2e35a628af30?searchText=triphenylphosphate Accessed on 7 August 2024

3.1.1.2 Oxidation

3.1.1.3 Phototransformation/photolysis

3.1.1.3.1 Phototransformation in air

Phototransformation in air for TPPT can be estimated by the QSAR program AOPWin v1.92 from EPI Suite (US EPA, 2012). OH-radical reactivity estimation is made up by reaction estimates of the OH-radical with aromatic rings and the thiophosphate group. These functionalities make up the whole of the TPPT structure. Twelve organophosphate compounds – of which 6 are thiophosphate esters – are present in the training dataset and used to calibrate the OH-radical reactivity towards the thiophosphate group. Therefore, the estimation of the AOPWin model can be considered well in domain and reliable. With a daytime of 12 hours per day and a default hydroxyl radical concentration of $1.5 \cdot 10^6$ per molecules per cm^3 during this period, the average daily half-life in air is 4.0 hours. However, the fugacity model of EPI Suite predicts the partitioning to air to be very low (<0.1%) and therefore this route of degradation is not expected to contribute significantly to the overall degradation of TPPT.

3.1.1.3.2 Phototransformation in water

No relevant information available.

3.1.1.3.3 Phototransformation in soil

No relevant information available.

3.1.1.4 Summary on abiotic degradation

Abiotic degradation is not expected to be a significant route of transformation in the environment for TPPT. An environmentally relevant aqueous half-life of 278 days at pH 7 and 12 °C has been extrapolated from an OECD TG 111 hydrolysis experiment on TPPT (Unpublished study report, 2007).

3.1.2 Biodegradation

3.1.2.1 Biodegradation in aqueous media or aqueous environment

3.1.2.1.1 Estimated data

BIOWIN v4.10 (US EPA, 2012) predicts the following values for TPPT:

Biowin1 (Linear Model Prediction): 1.28 (Biodegrades Fast),
Biowin2 (Non-Linear Model Prediction): 1.00 (Biodegrades Fast),
Biowin3 (Ultimate Biodegradation Timeframe): 2.66 (Weeks-Months),
Biowin4 (Primary Biodegradation Timeframe): 3.83 (Days),
Biowin5 (MITI Linear Model Prediction): -0.03 (Not Readily Degradable),
Biowin6 (MITI Non-Linear Model Prediction): 0.01 (Not Readily Degradable),
Biowin7 (Anaerobic Model Prediction): 0.59 (Biodegrades Fast).

It should be noted that the presence of a phosphate ester in all models has a significant positive contribution to the score for degradability. This phosphate ester contribution does not make a distinction between TPPT (thiophosphate) and TPP (phosphate), giving nearly identical QSAR estimates, in which the only difference between these groups is reflected by the difference in the molecular weight parameter of the prediction. However, from the hydrolysis tests (see Section 3.1.1.1. above) it follows that there is a clear distinction between triphenyl phosphorothioate and triphenyl phosphate if primary degradation due to hydrolysis is considered. Several phosphate esters, including the structurally closely related tricresylphosphate and cresyl-diphenylphosphate, are part of the training dataset, and the substructure fragments contributing to the degradation estimation cover the whole chemical structure of TPPT, therefore the BIOWIN model estimations can be considered well within the applicability domain. However, absence of any thiophosphate ester substances in the training dataset, and the indifference of the model towards the difference between the thio-phosphate and the oxo-phosphate (TPPT versus TPP) are indications that the BIOWIN estimates are not highly reliable, and most likely to give an overestimation (due to an overestimation of the phosphate ester group contribution to biodegradability) of the degradation potential of TPPT.

Based on the combination of the BIOWIN models 3 and 6, it could be concluded that more degradation relevant information is warranted, according to ECHA, 2023.

Inclusion of *tert*-butyl groups as substituents to the phenyl rings subsequently lowers the BIOWIN predicted values, indicating less biodegradation with increasing *tert*-butyl substitution. This seems to be confirmed in the ready biodegradability test results with TPPT and reaction mass of: triphenylthiophosphate and tert-butylated phenyl derivatives (see below).

3.1.2.1.2 Screening tests

Studies performed on TPPT

Several screening tests were performed for TPPT. In a modified Sturm test (OECD TG 301B), nonylphenol 10E05P0 was used as emulsifier to increase the bioavailability (Unpublished study report, 1988). The inoculum was from a non-adapted domestic sewage treatment plant in Rheinach, Switzerland. TPPT was applied in two concentrations of 10 and 20 mg/L. Blanks and blanks with emulsifier and reference substance (20 mg aniline/L) were included. The mineralisation of TPPT, measured as cumulative carbon dioxide production after 28 days, was 2 and 0%, in systems with 10 and 20 mg TPPT/L, respectively. The mineralisation of aniline was 94.4% after 28 days (Klimisch score 2).

Another modified Sturm test (OECD TG 301B) with lower concentrations of TPPT was performed in 2009 (Unpublished study report, 2009). The inoculum was from a domestic sewage treatment plant in Romanshorn, Switzerland. Included were test vessels with 0.26 µg/L of radiolabelled TPPT, inoculum blanks, a vessel with the reference substance sodium benzoate, and a toxicity control with 0.27 µg TPPT/L and sodium benzoate (tests contained 30 mg solids/L, 20 mg TOC/L), respectively. Mineralisation in the duplicates after 29 days was 19.3 and 17.8%. Analysis of the parent compound by HPLC-RAM showed that still 51.5 and 60.8% were present as TPPT after 29 days, this corresponds to 48.5 and 39.2% dissipation of the parent compound in 29 days. Mineralisation of the reference substance was 100% after 29 days (90.6% degradation after 14 days), confirming the microbial activity of the inoculum. The toxicity control showed 87.7% mineralisation after 14 days, indicating no inhibitory effects (Klimisch score 2).

A Zahn-Wellens test (OECD TG 302B) was performed with radiolabelled TPPT (Unpublished study report, 2008). Ethylene glycol was used as reference compound. The inoculum was from a domestic sewage treatment plant in Romanshorn, Switzerland, with a final concentration of 0.2 g solids/L in the test systems. Included were test vessels with 0.26 µg/L of radiolabelled TPPT, inoculum blanks, and a vessel with the reference substance (165 mg TOC/L), respectively. Mineralisation of ethylene glycol, based on DOC measurements, was 97.6% after 12 days and 98.2% after 28 days, showing the viability of the inoculum used. DOC was not measured for the test substance TPPT. Instead, total radioactivity was measured. For the test substance TPPT no filtration was performed as the samples from day 0 showed that all of the test substance was sorbed to the inoculum.

DOC measurements were consequently not possible. The recovery after 3.5 hours appeared to be 90%, which was attributed due to sorption, although this should not cause a decrease if LSC (liquid scintillation counting) is used. Radioactivity measured by LSC in the test after 28 days were 37.1 and 29.9% of the initial applied radioactivity. Compared to the value of 90% after 3.5 hours, this corresponds to a loss of 59.5 and 66.8% in the duplicates. This test has some deviations from the OECD TG 302B test protocol, because radioactivity instead of organic carbon was measured and not the dissolved but particulate phase was analysed. Because of the low solubility, the test set-up including DOC removal is in principle not suitable for this test substance. Further, radiolabelled test substance was used but no attempt for a mass balance was made (e.g. the mineralisation was not verified by measuring radiolabelled carbon dioxide). The dissipation of radioactivity indicates that significant transformation to volatile compounds (not necessarily CO_2) might occur under these conditions. Nevertheless, the observed losses do not meet the pass level of 70% removal of dissolved organic carbon within 7 days, according to R.11, v.4.0. (ECHA, 2023) (Klimisch score 4 because of too many deviations from test guideline).

Studies performed on reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives

A MITI-I test (OECD TG 301C) was performed with reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives EC 421-820-9 (Unpublished study report, 1999a). The inoculum was a mixture of sludge from ten different places in Japan. The sludge concentration in the tests was 30 mg/L. The concentration of the test substance was 100 mg/L. Aniline was included as reference substance but no further information on the degradation of the reference substance is given. Corrected oxygen consumption was negative (-5 to -7%) and consequently no mineralisation of the test substance was observed after 28 days. Analysis of the parent compounds by GC analysis showed 0% primary degradation for all seven compounds analysed (Klimisch score 2).

A closed-bottle test (OECD TG 301D) was performed with reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives EC 421-820-9 (Unpublished study report, 1996). Sludge was obtained from a non-adapted domestic sewage treatment plant in Godmanchester, UK. The inoculum used was prepared by settling of the sludge and subsequent filtration and 1 ml filtrate added to 1 L of test medium. The concentration of the test substance was 3 mg/L, applied on glass filter paper. Sodium benzoate was included as reference substance. A toxicity control containing both test substance and reference substance, and blanks with and without glass filter paper were also included. For each of the eight time intervals, separate bottles were sacrificed. No mineralisation, measured as oxygen consumption, of the test substance was observed (results varying from -6 to 4% with no trend over 28 days). The reference substance sodium benzoate was mineralised to 55 to 68% over all time points (degradation almost complete after 4 days). Toxicity controls were taken after 14 and 28 days and showed 66 and 67% mineralisation. The inoculum was biologically active and no inhibitory effects of the test substance occurred (Klimisch score 2).

3.1.2.1.3 Simulation tests

3.1.2.1.3.1 Biodegradation in water

A simulation test with TPPT in fresh surface water according to OECD TG 309 was performed (Unpublished study report, 2021a). Water was sampled from the surface layer (5 to 10 cm) of a pond near Hanhofen, Germany. Sediment taken from the sediment surface (5 to 10 cm) at the same location was added to the filtered water to achieve a total suspended matter concentration of 20 mg/L. As sediment was added to water, the test should be regarded as a suspended sediment test and not a pelagic test. The suspended matter concentration is at the lower end of the range for a suspended sediment test (OECD TG 309) and at the upper limit of what is considered still acceptable for a pelagic test, according to R.11, v.4.0. (ECHA, 2023). Higher suspended sediment concentrations might significantly enhance the biodegradability of the test substance. The water and sediment were sampled near the bank of the pond. It can be assumed that there is continuous interaction between the water and sediment at the sampling location.

The test was performed at 12 ± 2 °C in the dark and the system was equilibrated for 1 day. The test system was aerated under a constant flow of air and gentle orbital shaking. Oxygen levels were maintained. Each vessel contained 500 ml water. The pH after start of the test ranged from 8.1 to 8.4. Radiolabelled TPPT was used in nominal concentrations of 2 and 10 µg/L. TPPT was applied dissolved in acetonitrile, with the concentration of acetonitrile around 0.33‰. The test duration for the test with TPPT was 61 days, with sampling at 0, 2, 7, 14, 21, 29, 45 and 61 days. Duplicates were used for each sampling interval. A sterile control at 10 µg/L was also included. Radiolabelled sodium benzoate was used as reference substance. To the reference substance, the same amount of acetonitrile was applied. Analysis was performed by HPLC-MS/radio detection and TLC was used for confirmation.

Recovery from the test system was above 90%, except for one single replicate in the 10 µg/L group showing a recovery of 89%. Virtually no dissipation of TPPT occurred during the test. In both concentration levels, TPPT made up around 90% of the applied radioactivity at all time points. The half-lives thus exceeded the test duration by far (kinetics rate-constant for single first-order dissipation of the parent compound TPPT were 6.8E-15 and 0.00023 d^{-1} for the 2 and 10 µg/L groups, respectively; in both cases the lower limit of the 95% confidence interval for the half-life is exceeding 800 days). Production of carbon dioxide was limited and was not more than 4.0% and 4.3% in single replicates of the 2 and 10 µg/L groups, respectively. Moreover, it is plausible that this mineralisation is caused by a few impurities, which were present from the start of the test. In the sterile controls, sampled after 61 days, carbon dioxide was below 1% of applied radioactivity. As TPPT did not dissipate at all and the impurities did not accumulate, the impurities were not considered as degradation products. After 14 days, 83.4% of the applied radioactivity for the reference substance benzoate was mineralised, indicating that the test system was biologically active.

As there was no significant degradation, the added sediment apparently did not increase the degradation, and therefore the study is still relevant for the purpose of the persistence assessment. The test system is therefore considered reliable to assess the biodegradation in fresh surface water (Klimisch score 1).

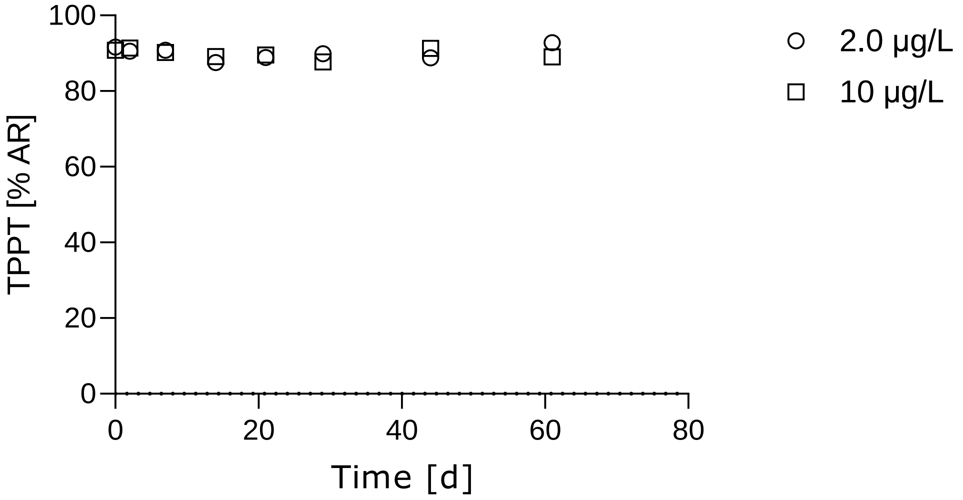

Figure 1: Dissipation of the parent compound TPPT in the OECD TG 309 simulation test.

3.1.2.1.3.2 Biodegradation in sediment

No relevant information available.

3.1.2.2 Biodegradation in soil

3.1.2.2.1 Simulation tests in soil

No relevant information available.

3.1.2.3 Summary and discussion on biodegradation

QSAR estimates indicate that TPPT would not be readily biodegradable, but could possibly be inherently biodegradable. The ready biodegradability test results are all negative, pointing at the potential persistence of the substance, even when low test concentrations were employed and high viability of and absence of toxic effects to the inocula were confirmed. One inherent biodegradability test showed relatively high dissipation of the test substance, but still the pass level for inherent biodegradability was not reached. Besides that, the validity of the obtained results could not be assessed sufficiently, due to deviations from the test guideline (OECD TG 302B).

A simulation study in fresh surface water was performed with TPPT according to OECD TG 309. While the reference substance showed high mineralisation in 14 days, the test substance was virtually not degraded over the test period of 61 days. It can thus be concluded that the half-life in fresh surface water is >>61 days.

3.1.3 Field data

No relevant information available.

3.1.4 Summary and discussion of degradation

QSAR predictions on biodegradation indicate borderline persistence for TPPT. Screening tests with either TPPT or reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives show that the substance is not readily biodegradable with mineralisation generally well below 20% after 28 days. In the simulation test on TPPT with natural pond water there was no indication of any significant degradation over the test duration of 61 days. Further, a hydrolysis test on TPPT showed that primary degradation by abiotic hydrolysis is a rather slow process. The outcome of the simulation test in water together with the results of the screening tests and the hydrolysis test, leads to the conclusion that TPPT is very persistent (vP).

3.2 Environmental distribution

3.2.1 Adsorption/desorption

One experimental study from 1997 in the registration dossiers of TPPT and EC 421-820-9[5] provides information on adsorption/desorption. The study is an OECD TG 121 HPLC estimation method, performed with reaction mass of: triphenylthiophosphate and its *tert*-butylated derivatives EC 421-820-9. The log K_{oc} value determined for the TPPT fraction of the mixture is 5.31. The log K_{oc} values of the butylated derivates of TPPT are much higher than 5.6 (Klimisch score 4, because log K_{oc} values of reference substances it not presented).

As supporting information, the QSAR estimation for TPPT of the log K_{oc} using the KOCWIN v.2.00 software (US EPA, 2012) is given in the registration dossier. The log K_{oc} estimation using the MCI method is 5.297, which is in line with the HPLC method. The log K_{oc} estimation using the log K_{ow} method, with the HPLC derived log K_{ow} in the registration dossier of 5.0, would be 3.6. This lower value, not in line with the HPLC derived log K_{oc} estimate, casts some doubt on the value of the log K_{ow} value of 5.00 as determined by the HPLC method. When the KOWWIN predicted value for log K_{ow} of 6.47 is used as input for the KOCWIN estimation program, a log K_{oc} of 4.41 is estimated. The MCI-based prediction model of the KOCWIN estimation program relies (only) on the training dataset of log K_{oc} values and the predictivity of the first order molecular connectivity index. The training dataset contains 10 aromatic organophosphorous compounds and 30 organo-thiophosphorous compounds, which contain either one (like TPPT) or two P=S fragments. The applicability domain of the MCI method therefore seems to cover substances like TPPT very well. A specific correction factor for thiophosphates is applied to the MCI-based prediction. The log K_{ow}-based model used by the KOCWIN estimation program directly uses the log K_{ow} estimation from KOWWIN and a relationship between log K_{ow} and log K_{oc}. In this case there is also a thiophosphorous specific fragment correction factor applied. Both models (MCI- and K_{ow}-based) therefore seem to be within the applicability domain and giving reliable predictions. The specificity of the MCI-based model combined with the high number of thiophosphorous compounds in the training dataset (30) as well as the possibility of polar/charge interaction with organic carbon matrices of the thiophosphate groups lead to the conclusion that for this case the MCI-based method yields the more reliable estimate of sorption to soil. For the risk assessment and fate modelling purposes the experimentally derived value for log K_{oc} of 5.32 (supported by the MCI-based KOCWIN estimate of 5.20) is considered best.

3.2.2 Volatilisation

The estimated Henry's law constant for TPPT calculated by QSAR using HENRYWIN v3.2 (US EPA, 2012) is 0.59 Pa.m^3/mol. The QSAR estimate can be reproduced using the bond-contribution model of the HENRYWIN QSAR. The Group contribution model in HENRYWIN is incomplete, as group contribution for the thiophosphate part of TPPT are missing. The group contribution estimate is therefore considered unreliable, but the bond-contribution model is considered sufficiently reliable as (like for all previously applied EPISuite model

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[5] Available at: https://chem.echa.europa.eu/

estimations) the substructure fragments contributing to the estimation (aromatic hydrogen-carbon bond, aromatic carbon-carbon bond, oxygen-phosphorous ester bond, phosphor-sulfur thiophosphate bond and aromatic carbon-oxygen bond) are completely describing the chemical structure of TPPT (no unknown bond contributions). In the training dataset up to 8 (pesticide) thiophosphate substances are present.

Henry's law constant can also be approximated by dividing the vapour pressure with the (molar) water solubility. Using the experimentally determined vapour pressure (0.0000136 Pa at 20 °C) and water solubility (0.020 mg/L at 20 °C) from the registration dossier this would yield 0.23 Pa.m^3/mol. As this is a simple approximation, and experimental determination of specifically the low vapour pressures for TPPT is inherently imprecise, the QSAR derived value for Henry's law constant is preferred. The values from both approached are close to each other, and the difference is not significant or relevant for the PBT-assessment.

3.2.3 Distribution modelling

The physicochemical properties of TPPT are used to estimate the distribution in the environmental compartments (Mackay level III fugacity model as included in EPI Suite (US EPA, 2012)). Assuming equal emission to air, water and soil, and using both an estimated log K_{ow} value of 6.47 (KOWWIN) as well as the HPLC-determined value of 5 given in the dossier, leads to the following distribution over the environmental compartments for TPPT:

	log K_{ow}=6.47	log K_{ow}=5.0
Atmosphere	0.1%	0.1%
Water	6.0%	5.7%
Soil	44.4%	43.0%
Sediment	49.5%	51.3%

3.2.4 Field data

No relevant information available.

3.2.5 Summary and discussion of environmental distribution

TPPT is very poorly biodegradable and is very slowly hydrolysed at environmental temperature and pH. The substance is not volatile and has a high log K_{oc}. TPPT will mainly distribute to soil and sediment compartments, with some distribution to water. Atmospheric degradation, as well as atmospheric transport, will not play a significant role in the fate of TPPT in the environment.

3.3 Data indicating potential for long-range transport

The atmospheric half-life of TPPT, predicted using with the AOPWIN estimation program v1.92 (US EPA, 2012) only estimates the half-life in the atmosphere (gas phase), using a conservative low average OH-radical concentration of $5 \cdot 10^5$ molecules/cm^3, to be 4 hours.

The fraction of TPPT sorbed to airborne particulates (phi) is estimated to be between 19.6 and 54.9% (using the log K_{oa} method and the Junge-Pankow, Mackay average method, AOPWin v1.92; US EPA, 2012). According to AOPWIN, the sorbed fraction may be resistant to the atmospheric oxidation. As a consequence, the atmospheric half-life in the gas phase of 4 hours is underestimating the total atmospheric half-life of TPPT (gas phase and particle phase).

The LRTP properties of TPPT have not been further evaluated (e.g. by running the OECD LRTP tool) and possible presence of TPPT in monitoring data, including monitoring data from remote areas like the Arctic or Antarctic, has not been investigated.

3.4 Bioaccumulation

3.4.1 Bioaccumulation in aquatic organisms (pelagic & sediment organisms)

3.4.1.1 Screening information for bioaccumulation of TPPT

The registration dossier of TPPT contains a log K_{ow} value of 5.0 estimated by the HPLC method (OECD TG 117). Also a value of 4.896 ± 0.395 is reported in the registration dossier, estimated by the QSAR Advanced Chemistry Development (ACD)/Labs Software V11.02, as well as a value of 6.5 (6.47) estimated by the KOWWIN (v1.67) module of EPI Suite v.4.0 (US EPA, 2012).

Other QSAR estimates are more in line with the value estimated by KOWWIN. BioLoom v.1.5 (Biobyte, 2006) predicts a value of 6.13, while ChemAxon's Marvin Sketch v. 16.10.24 predicts a value of 5.98 (Consensus model) or 6.33 (ChemAxon). COSMOTherm predicts a value of 6.97 at 20 °C for the log K_{ow} (Glüge and Scheringer, 2023). The more recent version of ACD Labs (v14.03) predicts a value of 5.45 (ACD/Labs, 2015), 0.45 log units higher than the one reported in the registration dossier. It can be concluded that the log K_{ow} of TPPT is well in excess of 4.5 and the substance screens as potentially B (ECHA, 2023).

As discussed earlier for the KOWWIN QSAR model (Section 1.5 Physicochemical Properties) the applicability domain of the KOWWIN model includes the complete TPPT structure, as plenty of thiophosphate compounds are present both in the training as well as the validation dataset of this model. As the QSAR models mentioned here for log K_{ow} all rely on roughly the same publicly available log K_{ow} data for their modelling purposes, it is likely that TPPT is in the applicability domain of those models as well. The overall trend is that TPPT is expected to have a significantly higher log K_{ow} than indicated by the experimentally estimated value of 5 using the HPLC method as referenced in the registration dossier. Given the consistently high estimates from the different QSAR models, one has to consider that TPPT is actually not in the applicability domain of the HPLC method (because of reference compounds that are not representative for TPPT) and that the QSAR estimates are more representative of the substance behaviour. For the PBT-assessment purposes we consider the range of 6-7 (5.98-6.97) as representative for the log K_{ow} of TPPT.

3.4.1.2 QSAR modelling of the bioconcentration factor for TPPT

In the TPPT registration dossier[6] several estimates of the bioconcentration factor (BCF) for TPPT are included. The QSAR based estimations all rely on the relationship between log

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[6] Available at: https://chem.echa.europa.eu/

K_{ow} and BCF, with possibly corrections for metabolism. For TPPT it seems likely that partitioning from water to fat (approximated by octanol-water partitioning) is the relevant mechanism leading to bioconcentration. Therefore the QSAR models relying on this relationship between BCF and log K_{ow} can be considered within the applicability domain for TPPT. The validity of the log K_{ow} value used as input in these QSAR models is a more relevant issue, including the applicability domain analysis for the determination (experimental or with QSAR) of the log K_{ow} value used. Correction for (possible) metabolism of a substance in the organisms should be compared to the very limited hydrolysis rate and almost absent biodegradation potential of the substance. Metabolism is less likely to become a large correction factor when the substance has a rather high stability in general.

The BCF calculated using Catalogic v.5.11.17 BCF base-line model v.02.09, according to the model by Dimitrov et al. (2005), is 2239 L/kg (log BCF = 3.35 ± 0.11), based on an experimental log K_{ow} of 5.0 with all mitigating factors (mainly correction for metabolism) applied. Without the mitigating factors the BCF is 5200 L/kg (log BCF = 3.716). TPPT is considered out of the structural domain of the Catalogic model, which indicates that structural features are present that were not sufficiently represented in the training dataset. Most likely this is due to the thiophosphate functionality. There are however no indications that a completely different mechanism for bioaccumulation could play a role for thiophosphate esters, so the relationship with log K_{ow} is still considered valid.

The BCF calculated using BCF model v1.0.2 implemented in the VEGA platform v1.0.8, according to the model by Meylan et al. (1999), is 11561 L/kg (log BCF = 4.06), based on a log K_{ow} of 7.12 as estimated by VEGA. The estimate is stated to be out of the applicability domain of the model.

The BCF predicted with BCFBAF v 3.01 of EPIWIN using the regression-based model, which is also based on Meylan et al (1999), and using the experimental log K_{ow} of 5, is 925 L/kg (log BCF = 2.97). With the Arnot-Gobas model a BCF of 643 L/kg (log BCF = 2.8) is calculated for the upper trophic level, including biotransformation estimate. Without biotransformation, a value of 7882 is calculated for this BCF. The estimated biotransformation half-life, calculated for a 10 g fish, is 1.669 days.

BCF calculated using T.E.S.T. (Toxicity Estimation Software Tool) v4.2.1 of US EPA was 216 L/kg. In the registration dossier, it is stated that "based on the mean absolute error (MAE), the confidence in the predicted BCF values is low". This indicates that the variability of the BCFs for the closest structural analogues in the training dataset is very large. This model estimation is therefore considered of low reliability.

The BCF calculated according to the read-across model VEGA Read-Across (version 1.0.2, implemented in the VEGA platform v1.0.8) is 136 L/kg (log BCF = 2.14). It is not mentioned which substances are considered most similar to TPPT and what BCF values for the read-across candidates were used for those substances.

The lowest BCF value of 98 L/kg (log BCF = 1.99) was calculated by the program VEGA CAESAR v2.1.13, implemented in the VEGA platform v1.0.8, based on calculated a log K_{ow} of 4.38 as calculated by VEGA-model. This log K_{ow} is almost 2 orders of magnitude below what is considered the most likely range of log K_{ow} values of 6-7.

These predicted values for BCF vary widely. Part of this can be attributed to variability in the log K_{ow} value used. Indeed, the lowest value is predicted with the lowest log K_{ow} value of 4.38 (VEGA CAESAR v.2.1.13) and the highest with the highest log K_{ow} of 7.12 (BCF Meylan Model v.1.0.2). If in the QSAR included in BCFBAF (US EPA 2012) the estimated log K_{ow} of 6.47 is used instead of the experimentally determined 5.0 consequently higher estimates for BCF, BAF and transformation half-life in fish result.

Overall, the QSAR estimates are considered inconclusive for bioaccumulation, but indicate the possibility that TPPT could exceed the B-criterion (BCF > 2000).

3.4.1.3 Aqueous BCF study with common carp performed with EC 421-820-9

A bioaccumulation study was performed with common carp (*Cyprinus carpio*) exposed to the reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives EC 421-820-9 (Unpublished study report, 1999b). The study was conducted to GLP following the Japanese test guideline "Bioaccumulation test of a chemical substance in fish or shellfish" provided in "the Notice on the Test Method Concerning New Chemical Substances".

At test initiation, the carp had an average weight of 26.4 ± 5.6 g and were 9.9 ± 0.6 cm long. The average lipid content of the carp was 4.3 ± 0.2%. The test was performed in a flow-through set-up with 100 L aquaria and a flow rate of 432 L/day. The dilution water was tap water. The test temperature was 25.1 ± 0.6 °C.

The test substance was applied at nominal concentrations of 0.5 and 0.05 mg/L. For the preparation of the aqueous solutions polyoxyethylene hydrogenated castor oil-based hydrophilic emulsifier with on average 20 EO units (HCO-20) was used as dispersant at a concentration of twice the test substance. The control contained the highest concentration of HCO-20 of 1.0 mg/L.

Twenty-five fish were kept in the aquarium with each of the test concentrations, and 6 in the control. Two fish were sampled on each occasion. Sampling was performed at exposure days 7, 14, 21, 28, 42 and 56, and additionally after 7 days of depuration. Water samples were taken at days 0, 7, 14, 21, 28, 35, 42, 49 and 56. Additionally, at day 49 two fish were sampled for analysis of several separate body parts. Control fish were sampled on days 0 and 56. Analysis was performed by GC-FID.

Analysis revealed that the aqueous concentrations were constant, with concentrations being very close to nominal. Peak 6 was not further quantified due to interferences in the GC chromatograms. For the six quantified peaks the average concentrations were between 90 and 105% of nominal. The main component, TPPT, was found during the exposure phase in concentrations of 0.180 ± 0.002 mg/L and 0.0183 ± 0.0004 mg/L for the high and low exposure group, respectively.

In the study report it is mentioned that the fish in the high concentration group showed swimming abnormalities from day 1, described as retrograding symptoms while swimming and symptoms of occasional convulsions, and fish did not recover at all from these symptoms after the 7-d depuration phase. Also food consumption was affected in the high treatment group. No such effects were observed at the lower concentration and in the control group containing only the emulsifier HCO-20. Effects on weight were not observed. In the control and in both concentration levels no increase of weight was observed and all weights were in the range of the initial weight, albeit that the variability of weights was rather high. All fish in the control and the low concentration group were reported to appear healthy throughout the entire test duration. Although the study report states that the fish were considered to be acceptable, toxic effects should be excluded according to OECD TG 305 and therefore, the data from the highest test concentration should be considered unreliable and should not be used to draw a conclusion on the bioaccumulation potential.

The concentration of TPPT in the lower concentration is above the lowest NOEC for rainbow trout (see section 5.1.1.2). OECD TG 305 stipulates that the test concentration should be below the chronic NOEC for the tested species. However, due to differences in sensitivity between fish species and between different life stages, the NOEC value will not be the same for all fish (in this case, the toxicity test has been performed with embryo/larval stages of rainbow trout while the bioaccumulation experiment has been performed with juvenile carp). Because no toxic effects are observed at the low concentration level on mortality, weight, food consumption, behaviour and general appearance, it is considered that this concentration level did not adversely affect the health status of the fish species tested in the bioaccumulation study. Furthermore, effects observed in the highest concentration level might as well be caused by physical effects due to the presence of undissolved substance instead of intrinsic toxicity of the dissolved components.

Concentrations of TPPT in fish increased up to the third week of exposure. From three weeks to seven weeks of exposure the concentrations were more or less constant at 323 ± 92 mg/kg in the high exposure group and 30.4 ± 6.6 mg/kg in the low exposure group, which can be considered as apparent steady-state. This leads to reported BCF_{SS} values of 1807 ± 511 (1274 – 2508) L/kg in the high concentration and 1645 ± 361 (1213 – 2194) L/kg in the low concentration. Based on this, the registration dossier concludes that TPPT has a BCF > 2000, but < 5000.

It should be noted that next to TPPT, also peaks 2 and 3, corresponding to mono-*tert*-butylated TPPT were found in fish. Measured concentrations in fish in the period of three to seven weeks were considerably lower than TPPT itself (peak 1) and were 6.7 ± 1.0 and 9.9 ± 2.0 mg/kg in the high exposure group and 0.90 ± 0.22 and 1.7 ± 0.5 mg/kg in the low exposure group, for peaks 2 and 3 respectively. Reported BCF values for peaks 2 and 3 for the period from 3 to 7 weeks were 83 ± 12 (63 – 103) and 77 ± 15 (51 – 101) L/kg in the high concentration and 106 ± 27 (64 – 148) and 124 ± 38 (75 – 182) L/kg in the low concentration, respectively.

In the study report and the registration dossier, BCF values were not normalised to a lipid content of 5%. Because the lipid content of the carp in the study was 4.3%, the normalised BCF values are accordingly higher. The lipid content was only measured at the start of the test, but in the absence of any significant growth during the test, it can be assumed that also the lipid content of the fish will have remained rather constant during the test, especially because the weight of all fish sampled during the entire test duration (27.1±5.6 g) is very similar to the reported initial weight of the fish (26.4±5.6 g). This leads to BCF_{SSL} values of 2101 ± 594 (1481 – 2916) L/kg in the high concentration and 1912 ± 420 (1410 – 2551) L/kg in the low concentration.

No kinetic modelling has been applied in the study. If a kinetic first-order model is applied to the data of the uptake phase, with the average measured water concentration over this period, the following results are obtained. High concentration: BCF_K = 2129 L/kg, k1 = 104.2 L/kg/d, k2 = 0.04894 /d (half-life 14.2 d), r^2 = 0.61. Low concentration: BCF_K = 1816 L/kg, k1 = 118.8 L/kg/d, k2 = 0.06543 /d (half-life 10.6 d), r^2 = 0.64. Normalised to 5% lipids, the BCF_{KL} values are 2476 and 2112 L/kg in the high and low concentration respectively. No growth correction is applied to these results as the carp did not significantly increase in weight during the test.

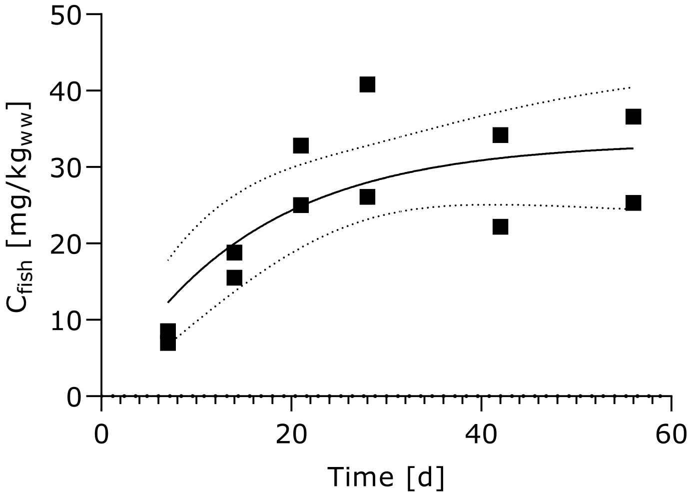

Figure 1: Uptake of TPPT in the low exposure concentration group. The solid line is the best fit of the first-order one-compartment model, while the dashed lines represent the 95% confidence interval of this estimate.

The depuration phase is limited to only one time point after 1 week of depuration. The depuration appeared to be remarkably high and not consistent with the relatively slow equilibration in the uptake phase. After one week of depuration, the concentration of TPPT in test fish were 25.9 and 124 mg/kg in the high exposure group and 0.271 and 0.0734 mg/kg in the low exposure group (which is at the x-axis in figure 1). Compared to the concentrations at 56 days of exposure estimated by kinetic modelling, these values are only 7 and 35% in the high concentration and 0.8 and 0.2% in the low concentration.

Several shortcomings were identified for the samples of the 7-d depuration time point. The low concentration is hampered by the fact that the concentrations are very close to the limit of quantification of 0.1 mg/kg for TPPT (this is also apparent from the fact that one of the duplicates has a peak area in the chromatogram that is 0.8 times the value of the other duplicate but the calculated concentrations is less than 0.3 compared to the other duplicate).

Furthermore, it appears that the calibration by means of two standard solutions deviated significantly on the analysis day for the depuration samples compared to the calibration of all other samples from the uptake phase, which is especially apparent in the high concentration. This may also have strong implications on the low concentration, as the offset of the calibration line was such that small positive peak areas resulted in a zero concentration.

Moreover, the half-life due to metabolism estimated by BCFBAF v3.01 (US EPA, 2012) using the predicted log K_{ow} value of 6.47 and extrapolated to 27-g fish is 6 d (k_{met} = 0.115 d^{-1}). Although one of the duplicates of the high concentration has a half-life that is comparable with this (4.6 d based on 35% left after 7 d), the other data and especially the duplicates in the low concentration show much faster depuration, making these values rather implausible (assuming that the depuration due to passive diffusion for a substance with log K_{ow} of 6.5 is orders of magnitude slower than this). In this sense, the k2 values obtained from the kinetic fit of the uptake phase are more in agreement with this estimate.

Also the fact that the fish in the high concentration did not recover at all from the behavioural symptoms is not an indication that the test substance is quickly removed from the body. Although toxic symptoms could be irreversible, sublethal toxic effects such as swimming behaviour are often quickly restored if the toxic component disappears, at least for (polar) narcosis, which is fully dependent on the internal concentration of the toxicant (McCarty & Mackay, 1993). The reported concentrations in fish for the high exposure group (0.7-1.3 mmol/kg wet weight; 15-31 mmol/kg lipids) are in the range that is lethal for substances that act by (polar) narcosis (as reported by McCarty et al., 1991 & McCarty & Mackay, 1993), which also explains the observed effects.

The study has been performed by dispersion of the substance in HCO-20 (polyoxyethylene hydrogenated castor oil-based hydrophilic emulsifier with on average 20 EO units) at a ratio of 1:2 (test substance: HCO-20 w/w). The fact that the bioaccumulation is performed in a mixture with non-soluble more hydrophobic components will also suppress the solubility of TPPT itself. For liquid mixtures (as the applied mixture in this study), this solution behaviour in water will be according to the theory of Raoult's Law. This means that the real dissolved concentration will be significantly lower than the aqueous solubility of TPPT, both in the high and in the low exposure group.

Raoult's Law has been successfully applied to calculate dissolved concentrations of individual components from complex organic mixtures in environmental relevant samples (e.g. Cline et al., 1991; Mukherji et al., 1997; Schmidt et al., 2002; Schluep et al., 2002; Sterling et al. 2003; Arp et al., 2011). Calculations with Raoult's Law have also successfully been applied for relating toxic effects to dissolved concentrations of individual components (e.g._McGrath et al., 2005; Verbruggen et al., 2008) and are e.g. also included in the PETROTOX model (Redman et al., 2012; 2017a). Toxicity (and consequently bioavailability) in such systems containing undissolved microdroplets is attributed to the dissolved concentrations of components of the mixture (Redman et al. 2012, 2017a,b).

Raoult's Law requires the calculation of liquid (subcooled) solubilities. This can be done in several ways. One is to calculate the solubility with WSKOW v1.41 (US EPA, 2012), setting the melting point to room temperature (25 °C). Another way is by a direct estimation from log K_{ow} (e.g. Verbruggen et al., 2008 based on ClogP (Biobyte, 2006) estimates). The subcooled liquid solubility is higher than the normal solubility at room temperature, because of the crystal energy for TPPT and other components: TPPT is a white crystalline substance while reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives is a liquid. The estimated subcooled liquid solubilities of TPPT are 88 and 98 µg/L, determined by both methods respectively, which is in good agreement with the experimentally determined solubility of ~0.1 mg/L for TPPT as the main component in reaction mass of: triphenylthiophosphate and tert-butylated phenyl derivatives (see Table 6).

The real dissolved concentrations can be calculated by numerically solving the aqueous concentrations of all constituents of the substance together, so that the distribution over the two phases fulfills Raoult's law (Verbruggen et al., 2008): $C_{w,i} = x_i * S_{L,i}$
In this equation, $C_{w,i}$ is the molar aqueous concentration of constituent i, x_i is the mole fraction in the organic phase and $S_{L,i}$ is the molar aqueous (subcooled) liquid solubility. The ratio of $C_{w,i}$ and x_i indicates how much of the constituent is dissolved in water.

Both methods were applied to estimate the dissolved concentration of TPPT from the nominal concentrations and the given composition of the tested UVCB. The dissolved TPPT concentrations in the nominal concentration of 50 µg/L are 13.2 and 13.6 µg/L, corresponding to 75% and 77% of the nominal concentration of TPPT being dissolved. If the influence of the dispersant HCO-20 is also taken into account (assuming an average molecular weight of 1814.53 g/mol and negligible solubility) the concentrations are further reduced to 11.2 and 11.6 µg/L, corresponding to 64% and 66% of the nominal concentration of TPPT being dissolved.

The dissolved fraction should be considered most relevant for bioaccumulation in fish, as undissolved colloidal material will be merely unavailable for uptake (Redman et al., 2012, 2017a,b). This means that the measured (total) concentrations, which are close to nominal, should be considered as a substantial overestimation of the real exposure concentrations, and thus the bioconcentration factors, which are very close to the B criterion of 2000, should be substantially higher as well and could even be higher than the vB criterion of 5000.

The study is assessed as Klimisch score 2 for the low exposure concentration and Klimisch score 3 for the high exposure concentration and the depuration phase.

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

KOAWIN v. 1.10 of the EPI Suite (US EPA, 2012) predicts a log K_{oa} of 10.09 for TPPT. The KOAWIN estimation fully relies on the (estimated) octanol-water and water-air (Henry) partition coefficients. For both, the KOWWIN QSAR as well as the HENRYWIN QSAR, the substance TPPT was considered within the applicability domain and giving a reliable estimate. Therefore also the log K_{oa} estimate based on the estimated log K_{ow} (6.47, KOWWIN v1.68) and log K_{aw} (-3.624, HENRYWIN v3.20, unitless, equal to the (estimated) Henry's law constant of 0.59 Pa.m3/mol) is considered within the applicability domain of the QSAR model and giving a reliable estimate.
Since TPPT has a log $K_{ow} > 2$ and a predicted log $K_{oa} > 5$, it screens as bioaccumulative in air-breathing organisms (ECHA, 2023).

3.4.3 Field data

No relevant information is available

3.4.4 Summary and discussion of bioaccumulation

The bioaccumulation study performed with carp exposed to reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9) shows TPPT bioconcentration factors close to or exceeding 2000, based on the low exposure test concentration which is the reliable part of the study (Klimisch 2). Normalised to 5% lipids, kinetic BCFs based on the data from the uptake phase are in excess of 2000. The data for the depuration after one week in this test are considered not reliable. Furthermore, the bioavailability of TPPT is reduced in this test due to the application together with its tertiary butylated phenyl derivatives. These data together are considered enough to conclude that TPPT at least meets the B criterion (BCF > 2000).

TPPT is considered to have a lipid normalised kinetic BCF_{KL} around 2112 L/kg (low tested concentration). TPPT therefore meets the B-criterion for the PBT-assessment.

3.5 Summary and discussion of environmental fate properties

TPPT is expected to be very persistent in the aqueous environment based on the biodegradability and hydrolysis test results. Atmospheric degradation due to abiotic reaction with OH-radicals is estimated to be relatively fast (daily average t1/2 of 4 hours), but as the substance is not volatile, atmospheric degradation is not considered to be a significant removal route. TPPT is bioaccumulative in fish.

4. Human health hazard assessment

Not evaluated

5. Environmental hazard assessment

5.1 Aquatic compartment (including sediment)

5.1.1 Fish

5.1.1.1 Short-term toxicity to fish

Studies performed on TPPT[7]

An acute toxicity study from 2002 with zebrafish (*Danio rerio*) according to OECD TG 203 exposed fish for 96 hours to a saturated solution of TPPT, which was prepared by dispersing 100 mg/L and subsequent filtering over a 45 µm filter. No analysis of actual concentrations was performed. No toxic effects were observed, some undissolved material was observed in the test vessels after 24 hours (Klimisch score 3).

In another acute toxicity test with zebrafish from 1988 according to OECD TG 203, fish were exposed to a series of 8 concentrations of TPPT ranging from 1.8 to 100 mg/L for 96 hours. A dispersant/solvent was used to prepare the test solutions. The solvent control contained the concentration used to prepare the highest concentration. This contained 432.8 mg/L 1-methyl-2-pyrrolidon and 0.8 mg/L alkylphenol-polyglycol-ether. The observed LC50 was 83 mg/L. Also, in this test undissolved material was visible after 24 hours in the three highest concentrations in the range of 32 to 100 mg TPPT/L. These were also the concentrations at which mortality occurred (Klimisch score 3).

Studies performed on reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives[8]

In a test from 1997 performed with zebrafish according to OECD TG 203, the water accommodated fraction from the 100 mg/L filtrate was diluted to nominal concentrations of 6.25, 12.5, 25 and 50 mg/L. Further, the test solutions were renewed after 48 hours. In this test no mortality occurred. The test substance refers to the reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9) as can be seen from the inactive registration dossier on this substance (Klimisch score 3).

In the bioaccumulation study with reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9), a range-finding test was also performed. Killifish (*Oryzias latipes*) were exposed for 48 hours to this test substance (Unpublished study report, 1999b). Similar to the bioconcentration tests, HCO-20 was used as a dispersant in an amount twice that of the test substance. Concentrations were analytically verified and ranged from 2.8 to 78.4 mg/L. Mortality occurred at the three highest concentrations ranging from 30.6 to 78.4 mg/L. The reported LC50 for the test substance was 35 mg/L (Klimisch score 3).

In conclusion, all acute toxicity tests with fish have been performed with concentrations that well exceed the water solubility of TPPT, applied either as single constituent or as constituent in reaction mass of: triphenylthiophosphate and tertiary butylated phenyl

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[7] Available at: https://chem.echa.europa.eu/

[8] Available at: https://chem.echa.europa.eu/

derivatives. In the tests that used dispersants or solvents, mortality was observed at high concentrations, in contrast to the tests with water accommodated fractions. Analytical monitoring was lacking in the two tests performed on TPPT. In general, the relevance and reliability of these tests is low.

5.1.1.2 Long-term toxicity to fish

Study performed on TPPT

A fish early life-stage study according to OECD TG 210 was performed with rainbow trout (*Oncorhynchus mykiss*) exposed to TPPT (high purity of 99.9%) under flow-through conditions (Unpublished study report, 2023). The test duration was 97 d (60 d post-hatch). A preliminary test was also run with a test duration of 75 d (41 d post-hatch). The test water was laboratory well water with a temperature between 9.5 and 11 °C, and a pH between 6.5 and 7.1. The hardness was between 64 and 71 mg $CaCO_3$/L. Total organic carbon of the dilution water was between 0.54 and 0.82 mg/L.

Aqueous concentrations were prepared by saturator columns. The preliminary test consisted of controls, and nominal test concentrations of 0.1, 1, and 10 µg/L. In the final test, next to controls, the nominal test concentrations were 0.26, 0.64, 1.6, 4.0 and 10 µg/L. During the test duration, samples for each concentration level were taken at 42 occasions, alternating between the four replicates per concentration. Chemical analysis was performed by GC-MS/MS. Time-weighted average measured concentrations were close to nominal and were 0.26, 0.67, 1.7, 4.3 and 12 µg/L. Testing started when the embryos were approximately 2 h old. The test started with 40 embryos per replicate in an incubation cup. The embryos were thinned to 20 on day 22 of incubation, while the remaining embryos of the replicate were held in a second incubation cup until hatching to assess overall hatching success. The larvae of the group of 20 were transferred on day 37 to aquaria, when hatching was complete in all replicates except one in the 4.3 µg/L group. After this transfer were exposed for another 60 days. The larvae were fed live brown shrimp nauplii from 9 days post-hatching on (day 46 of the test).

In the preliminary test, the embryo hatching was low (61% in the controls and 61, 61 and 66% in the exposure groups respectively) and did not meet the quality criterion (75 % as minimum). However, the test provided robust information for selection of the concentration in the definitive test. Hatching success, normal larvae at hatching and mean time to hatch were not affected in any of the treatment groups compared to the control. However, all larvae died in the highest concentration of 10 µg/L, while the mean time to swim up, survival, length and weight at the end of the test was unaffected in the 0.1 and 1.0 µg/L groups compared to the controls.

In the definitive test, there were no significant effects on hatching success (85-91%) and there were also no effects on the number of live, normal larvae (99-100%). Mean days to hatch was 31 days in all groups. Mean days to swim up was 47 days in all groups except the highest concentration where it was 48 days. This was considered significantly different. The most sensitive endpoint appeared to be the post-hatch survival of the larvae (exposed for 60 days after hatching was complete). The NOEC for this endpoint was stated to be 1.7 µg/L, with the LOEC being 4.3 µg/L. The survival was 100, 98, 98, 95, 27, and 0% for control, 0.26, 0.67, 1.7, 4.3 and 12 µg/L, respectively. The 95% survival in the 1.7 µg/L was statistically different from the control, but considered as not biologically relevant. For the treatment groups without high mortality (0.26, 0.67 and 1.7 µg/L) the length and weight of the larvae at test termination were not significantly different from the controls.

It is stated in the study report that dose-response modelling is not possible due to a lack of fit for the non-linear models. It appears that dose-response relationships are very steep, which may hamper the curve fitting. However, the data for the larval survival in the 60-d post-hatching period fit a log-logistic dose-response relationship very well (r^2=0.9997). The EC10 and EC50 derived from these data are 2.1 and 3.5 µg/L, respectively. Similarly, for the reported overall survival (i.e. survival from viable embryos to test end) a log-logistic dose-response relationship can be fitted to the data. The overall survival was 85, 87, 88, 84, 24, and 0% for control, 0.26, 0.67, 1.7, 4.3 and 12 µg/L, respectively. The outcome is almost the same as for larval survival (EC10 and EC50, 2.2 and 3.5 µg/L, respectively; r^2=0.9994; see Figure 2). This also shows that the effects become manifest in the second part of the study. The fitted EC10s and EC50s are well in accordance with the NOEC and LOEC as indicated in the study report. The study is assessed as Klimisch score 1.

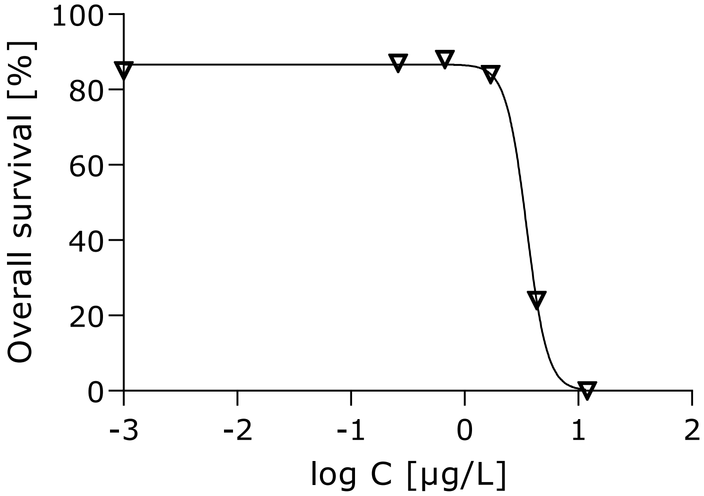

Figure 2: Overall survival of rainbow trout embryos and larvae exposed to TPPT

Study performed on reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives

An earlier OECD TG 210 study with rainbow trout was performed with reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9) (Unpublished study report, 2003a). In this study, the test material was applied dissolved in dimethyl formamide (DMF) in a flow-through set-up. The final concentration of DMF was 0.1 ml/L. Control and solvent controls were included in the test. The test duration was 87 d (60 d post-hatch). Nominal concentrations of the test material were 6.3, 13, 25, 50 and 100 µg/L.

Analytical monitoring was done by GC-FPD. Analysis of the test material was based on two main peaks. The chromatogram of the substance looks very similar to the chromatograms from the bioconcentration study (see section 3.4.1). It is therefore likely that the two constituents that form the basis for the analysis are TPPT and one of the mono-substituted *tert*-butyl derivatives of TPPT. The analysis was conducted at least once a week. The mean measured concentrations were 4.4, 8.7, 17, 29 and 66 µg/L, expressed as test substance. Based on the content of TPPT in the UVCB, these concentrations correspond to 1.3, 2.6, 5.2, 8.8 and 20 µg/L.

Hatching success was not affected in the exposure groups (78-86%). Also, the time to hatch was not affected in any of the treatment groups (23-27 days). Time to swim-up was significantly affected in the 17 µg/L group, while in the two highest treatment groups no larvae reached swim-up status. Swim-up percentages on day 16 post-hatching were 91% in the control and solvent control and 94, 92 and 30% in the 4.4, 8.7 and 17 µg/L groups, respectively. Larval survival until day 16 post-hatching was not affected. At this day larvae were thinned to 15 per group (no information is given how the larvae were selected).

However, larval survival from day 16 to day 60 post-hatching was significantly reduced at 17 µg/L. The survival was 100% in the control and solvent control groups and 100, 97 and 53% in the 4.4, 8.7 and 17 µg/L groups, respectively. None of the larvae of the two high dose groups achieved swimming and all of the selected, most active, larvae had died by day 29 post-hatch.

The length and weight of the larvae in all exposure groups was significantly reduced compared to the pooled controls. However, compared to the solvent control only, the length and weight were not significantly different in the lowest concentration of 4.4 µg/L at study termination. It is stated in the report that the observed statistical difference is due to outliers in the controls and solvent controls. However, a re-evaluation of the study showed that significant outliers in the control and solvent control could only be detected by Grub's test for wet and dry weight, but not for length at both time points (29 and 60 days post-hatch). Besides that, length at post-hatch day 29 is also significantly delayed at 4.4 µg/L compared to the solvent control group. It can be concluded that some effects on growth (length/weight) were observed, for which the NOEC lies below the toxicity criterion of 10 µg/L.

No dose-response modelling was applied in the report. However, also in this case, log-logistic dose-response modelling fits the reported data for percentages larvae that reached the swim-up stage (by day 16 post-hatch) and percentage survival of larvae after thinning (from day 16 to 60 post-hatch). For percentage swim-up, the EC10 and EC50 are 15.4 and 16.6 µg/L, respectively (r2=0.9995). For larval survival after thinning, the EC10 and EC50 13.8 and 17.2 µg/L, respectively (r2=0.9995). Overall survival (from embryo hatching to test end) is not reported in this study, but if it is calculated in the same way as done in the new ELS study (OECD TG 210) with TPPT described above (Unpublished study report, 2023), the percentages overall survival are 79, 79, 75, 82, 43, 0 and 0% in the control, solvent control, 4.4, 8.7, 17, 29 and 66 µg/L groups, respectively.

Although the dose-response modelling is hampered by the steep-dose response, it is clear that the EC10s are between the concentrations of 8.7 and 17 µg/L, while the EC50s are around the concentration of 17 µg/L. If the toxicity of the mixture would be fully attributed to TPPT, the effect concentrations for larval survival would be 4.2 and 5.2 µg/L for the EC10 and EC50 respectively, i.e. slightly higher than observed in the test with pure TPPT.

In the test with the UVCB, not all of the test substance will be dissolved. This presence of an undissolved phase is also confirmed by the study report that mentions the observation of a slight oily surface film in the diluter mixing chambers, increasing with concentration. This could also reduce the bioavailability of TPPT, when administered as a mixture, due to the presence of more hydrophobic undissolved components (see also the discussion on bioaccumulation on the solubility of TPPT applied in a mixture in Section 3.4.1.3 above). The dissolved concentrations of TPPT are calculated from the nominal concentrations of the test substance with Raoult's Law and the specific composition for this test substance (see section 3.4.1.3 for details on the calculation method). The resulting dissolved concentrations of TPPT are 1.8, 3.5, 6.5, 11 and 17 µg/L (based on WSKOW estimates (US EPA, 2012), 1.8, 3.5, 6.6, 12 and 18 µg/L, based on regression with log K_{ow} values estimated by ClogP (BioByte, 2006), see also 3.4.1.3 for further details). For the lower three concentrations, the estimated undissolved part will be ≤14%. Based on estimated dissolved TPPT concentrations, the EC10 and EC50 for percentage swim-up are 6.0 and 6.4 µg/L, respectively. The EC10 and EC50 for larval survival after thinning are 5.2 and 6.7 µg/L, respectively.

In conclusion, the test (OECD TG 210) performed with reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9) (Unpublished study report, 2003a) supports the results of the test (OECD TG 210) performed with TPPT alone ((Unpublished study report, 2023) , which shows slightly lower effect concentrations. Although in the test with EC 421-820-9 small contributions due to the presence of the

other constituents (mono-*tert*-butylated and di-*tert*-butylated TPPT) cannot be ruled out, it seems likely that the toxic effects observed are mainly caused by TPPT, as the solubilities of other constituents are expected to be extremely low. For example, the calculated log K_{ow} value for mono-*tert*-butylated-TPPT is 8.38 (almost 2 log units above the value of 6.46 calculated for TPPT), and for di-*tert*-butylated-TPPT a value of 10.28 (another 2 log units more) is estimated. These very high log K_{ow} values indicate extreme low solubility, roughly a factor of 100 (2 log units) or 10000 (4 log units) less than for TPPT.
The study reliability is assessed as Klimisch score 2.

5.1.2 Aquatic invertebrates

5.1.2.1 Short-term toxicity to aquatic invertebrates

Studies performed on TPPT[9]

In an acute toxicity study from 2002 according to OECD TG 202, neonate daphnids (*Daphnia magna*) were exposed for 48 hours to a saturated solution of TPPT, which was prepared by dispersing 100 mg/L and subsequent filtering over a 45 µm filter. No analysis of actual concentrations was performed. No toxic effects were observed (Klimisch score 3).

In another acute toxicity test from 1988 with *Daphnia magna,* according to OECD TG 202, daphnids were exposed for 24 hours to TPPT a series of 5 concentrations of TPPT ranging from 10 to 100 mg/L. A solvent was used to prepare the test solutions. The solvent control contained the concentration used to prepare the highest concentration. This contained 159.8 mg/L dimethyl formamide (DMF) and 1 mg/L alkylphenol-polyglycol-ether. The observed EC50 was 49 mg/L. Undissolved material was visible after 24 hours in all concentrations (Klimisch score 3).

Studies performed on reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives[10]

In an OECD TG 202 test from 1996 performed with *Daphnia magna*, the water accommodated fraction from the 100 mg/L filtrate was diluted to nominal concentrations of 21 and 45 mg/L (and 1, 10, and 100 mg/L in a range-finding test). Semi-quantitative analysis was performed, but not used for effect concentrations. Also in this test no effects were observed (Klimisch score 3).

In conclusion, all acute toxicity tests with daphnids have been performed with concentrations that well exceed the water solubility of TPPT. In the test that used solvents, mortality was observed at high concentrations, in contrast to the tests with water accommodated fractions. Quantitative analytical monitoring was lacking in all tests. In general, the relevance of these tests is low.

5.1.2.2 Long-term toxicity to aquatic invertebrates

Studies performed on TPPT

A reproduction test with <24-h old *Daphnia magna* according to OECD TG 211 was performed with TPPT (high purity of 99.9%) under static-renewal conditions (Unpublished study report, 2021b). Adult daphnids were individually exposed in beakers containing 50

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[9] Available at: https://chem.echa.europa.eu/

[10] Available at: https://chem.echa.europa.eu/

ml test solution. The test duration was 21 d. The test water was synthetic medium (Elendt M4) with a temperature between 19.5 and 20 °C, and a pH between 8.0 and 8.2. The hardness was 22 mg $CaCO_3$/L. The daphnids were fed with algae (*Desmodesmus subspicatus*) in an amount of 0.1-0.2 mg total organic carbon per daphnid per day (i.e. 2-4 mg TOC/L).

The test was performed as a limit test. A saturated solution was prepared by coating the substance to the wall of a glass bottle by applying it in acetone followed by complete evaporation of the acetone. Next, the medium was equilibrated in the bottles by stirring it for 24 hours. It is stated in the test report that test solutions were renewed daily, although from the reported analyses (pH, hardness, temperature, chemical analyses) as well as from the impact of the volume of feeding (2-3 times the daily volume), it can be concluded that renewal was once every two to three days with nine renewals over the test duration. The concentrations were analysed in the freshly prepared solutions, in the test vessels just before renewal and in abiotic controls just before renewal (i.e. test vessels without daphnids and algae). Chemical analysis was performed by GC-MS/MS (LOQ = 2 µg/L).

For the time-weighted average concentrations, the measured concentration in the freshly prepared solutions and in the abiotic control before renewal were used. This was done, because the concentrations in abiotic controls were ≤ 20% lower than in the freshly prepared solutions. As a matter of fact, the concentrations in the aged abiotic controls (on average 7.32 µg/L) were slightly higher than the concentrations in the freshly prepared solutions (on average 7.04 µg/L), which shows that the concentration in the test vessels is not lowered by abiotic losses and/or (bio)degradation. The calculated time-weighted average concentration used in the test is 7.24 µg/L. However, both the freshly prepared solutions and the abiotic controls do not represent the solutions the daphnids have been exposed to (no algae added in both cases). In the test report, it is stated that the low measured values in the biotic samples before renewal are most likely due to the test substance binding to the increased amount of food (algal cells) used in the later days of the test, a statement which seems plausible. Because algae were added just after renewal, the average concentration measured in the biotic samples before renewal might represent the time-weighted exposure concentration of the daphnids, as other processes than the addition of algae and daphnids did not seem to lower the concentration. The time-weighted average concentration of the biotic samples could be calculated from the data in the report to be 3.9 µg/L.

All validity criteria were met (no parent mortality and the average number of living young per parent was 124 in the controls). None of the endpoints showed a significant effect compared to the control. The average number of living young per parent was 126±20 in the exposed group versus 124±16 in the controls. No parent daphnids died in the exposed group either. The length of the parent daphnids at the end of the test duration was 4.28±0.13 mm in the exposed group, while it was 4.27±0.13 mm in the control groups. The time to first brood was 9.2±0.6 days in the exposed group, while it was 9.4±0.8 days in the control groups. All these effects showed no signs of toxicity at the single concentration tested. In the study report the NOEC is mentioned as ≥7.24 µg/L. However, based on the measured concentrations in the exposure solutions, this should better be expressed as ≥3.9 µg/L (Klimisch score 2).

Studies performed on reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives

Further, two chronic toxicity studies for *Daphnia magna* conducted with reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9) are available.

The more recent semi-static *Daphnia magna* 22-d reproduction study according to OECD TG 211 (Unpublished study report, 2015) was conducted as a limit test at a nominal concentration of 5.5 mg/L without application of a solvent, in synthetic test medium (Elendt M4). Following 3 days of stirring at room temperature and subsequent filtering, the undiluted filtrate was used as test medium. Test solutions were renewed daily with freshly prepared solutions. Daphnids were fed with algae on a daily basis in amounts of 0.1 to 0.2 mg TOC per animal per day. The validity criteria were met, and no adverse effects on mortality, reproduction, growth or behaviour were observed. A NOEC for reproduction of >5.5 mg/L was reported based on nominal test concentration.

Analytical monitoring was based on two main constituents, which were not further identified. Analysis was done by GC-MS, with m/z of 383.10 and 398.10, which implies that the measured peaks correspond to mono-*tert*-butyl triphenyl phosphorothioate isomers and that TPPT itself (Mwt of 342.35 g/mol) is not among the measured peaks. Only two peaks are visible in the chromatograms (similar to the number of peaks for mono-*tert*-butyl triphenyl phosphorothioate isomers described in the bioaccumulation study, section 3.4.1 above), with the second peak being about 6 times higher than the first peak. Concentrations of the test substance were expressed as total mass of the test substance based on regression of the peak area of each peak with the total mass of the test substance. Analysis by either one of the peaks yielded very similar values for the total concentration of the test substance in each sample. This implies that both peaks represent substances that are dissolved to approximately the same extent in the water accommodated fraction, thus further confirming the similarity of the peaks.

Analysis was conducted at test start, and subsequently once a week for freshly prepared, aged and control solutions. The test substance was detected in quantities around the LOQ of 0.2 µg/L in two aged control samples (non-exposed daphnids) at day 9 and 18. In the treatment, the actual concentrations were very low and varied strongly between batches. During the first two days, no reliable concentrations could be determined, because the concentrations of both constituents were below the LOQ of 0.2 µg/L in all samples. Subsequent measurements from day 8 to day 18 ranged from 0.78 to 3.6 µg/L, i.e. not higher than 0.066% of the initial loading, but exceeding the solubility of mono-*tert*-butyl triphenyl phosphorothioates (~0.2 µg/L by WSKOW v1.41 from EPI Suite (US EPA, 2012)).

In the study report, it is mentioned that low concentrations can be expected as the aqueous solubility of UVCB substances is highly dependent on the loading rate and test medium composition. The presence of other constituents could have reduced the water solubility of TPPT (as also discussed above in section 3.4.1 for bioaccumulation). Because TPPT is not measured in this study and because exposure concentrations of other constituents were highly variable, the relevance and reliability of this test for the assessment of the toxicity of TPPT should be considered as low, even though no effects were observed (Klimisch score 3).

The second *Daphnia magna* 21-d reproduction study performed according to OECD TG 211 was conducted under flow-through conditions using five nominal test concentrations of reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9) ranging from 6.4 to 250 µg/L (Unpublished study report, 2003b). The water used was moderately hard well water with a pH ranging from 8.2 to 8.4 during the test. Per treatment group, 20 neonate daphnids divided over four replicates were used. Daphnids were fed with a mixture of yeast, Cerophyll®, and trout chow, as well as a suspension of the freshwater green alga, *Selenastrum capricornutum*, three to four times per day. The total amount fed is not mentioned in the report. Dimethyl formamide (DMF) was used as solvent. The solvent concentration amounted to 0.08 mL/L, which is in accordance with OECD TG 211. Validity criteria for the test were met.

Analytical monitoring was done by GC-FPD. The two constituents that form the basis for the analysis probably are TPPT and one of the mono-substituted *tert*-butyl derivatives of TPPT (see also section 5.1.1 on the ELS test with rainbow trout performed with the same test substance). The analysis was conducted at least once a week. The mean measured concentrations, expressed as test substance, were reported to be 4.9, 11, 26, 46 and 150 µg/L. Based on the content of TPPT in the UVCB, these concentrations correspond to 1.5, 3.3, 7.9, 14 and 45 µg/L.

Parent mortality at the end of the test in the control, solvent control and nominal concentrations of 4.9, 11, 26, 46 and 150 µg/L was 90, 85, 75, 95, 85, 65 and 65%, respectively. The length of the parent daphnids at the end of the test was 4.60, 4.52, 4.54, 4.55, 4.55, 4.54 and 4.07 mm, while the dry weight was 1.14, 0.92, 0.93, 0.88, 0.83, 0.91 and 0.61 mg in the control, solvent control and nominal concentrations of 4.9, 11, 26, 46 and 150 µg/L, respectively. The mortality in the two highest concentrations was significantly different from the pooled controls. Statistically lower growth (both length and dry weight) was observed for the highest concentration only. The average number of young per reproductive day were 6.43, 7.97, 8.38, 7.76, 8.57, 8.64 and 5.79 in the control, solvent control and nominal concentrations of 4.9, 11, 26, 46 and 150 µg/L, respectively. None of the concentrations showed a statistically significant effect. However, in the report, it is mentioned that it cannot be precluded that the lower value in the highest concentration with 20% decrease in reproduction is the onset of an effect. The most sensitive NOEC of 26 µg/L, expressed as test substance, was for mortality of parent daphnids, which corresponds to 7.9 µg TPPT/L.

Test solutions were prepared by delivering primary or secondary stock solutions in DMF to diluter mixing chambers, where mixing with the test medium yielded the desired test concentrations. The report states that an oily film was observed in the diluter mixing chambers of the treatments, which indicates water solubility issues. If the concentrations are calculated from the nominal concentrations of the test substance with Raoult's Law and the specific composition for this test, the dissolved concentrations of TPPT were 1.9, 4.4, 9.5, 17 and 24 µg/L (based on WSKOW estimates (US EPA, 2012), 1.9, 4.4, 9.7, 18 and 26 µg/L, based on regression with log K_{ow} values estimated by ClogP (BioByte, 2006), see also 3.4.1.3 for further details). On this basis, the NOEC would be 9.5-9.7 µg TPPT/L.

The data from the flow-through test with the UVCB substance tested indicate that the chronic toxicity for *Daphnia* magna might just meet the T criterion for TPPT, because effects are observed at estimated concentrations of 7.9-9.7 µg/L. The observed absence of effects at the second test concentration (3.3-4.4 µg/L) are in accordance with the limit test for the pure substance (NOEC ≥3.9 µg/L). Nevertheless, as other substances were present in the test medium at low concentration, it is not possible to fully address the observed toxicity in the tests with the UVCB to TPPT only. (Klimisch score 2).

5.1.3 Algae and aquatic plants

Studies performed on TPPT

An algae growth inhibition test according to OECD TG 201 was performed with the freshwater algae *Desmodesmus subspicatus* for a test duration of 72 h (Unpublished study report, 2013). The test substance was TPPT with a purity of 99.8%. The study was conducted as a limit test. A nominal loading of 100 mg/L without application of a solvent was stirred for 3 days at room temperature and subsequently filtered over a 0.45 µm membrane filter. The undiluted filtrate was used as test medium. No suitable analytical technique was available and therefore, the exposure concentrations are unknown. If the substance was dissolved up to the solubility limit, filtration and addition of algae may have had an impact on the dissolved concentrations. The validity criteria of the test were met, and no inhibition of growth rate was observed. Since no toxic effects were observed, the NOEC would ordinarily be expressed as equal to or above water solubility. However, in this case the procedure followed to dissolve TPPT might have resulted in an unknown lower exposure concentration (Klimisch score 3).

Studies performed on reaction mass of: triphenylthiophosphate and tertiary butylated *phenyl derivatives*

An earlier study according to OECD TG 201 was performed with the freshwater algae *Desmodesmus subspicatus* for a test duration of 72 h with reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9) (Unpublished study report, 1997). Also, in this case no effects were observed. An attempt was made to analyse the different constituents, but TPPT and tert-butylated derivatives could not be measured, resulting in the fact that the actual exposure concentration remains unknown (Klimisch score 3).

5.1.4 Sediment organisms

No relevant information available.

5.2 Terrestrial compartment

5.2.1 Toxicity to soil macro-organisms

In the registration dossier of reaction mass of: triphenylthiophosphate and *tert*-butylated derivatives, a chronic toxicity test (56 days) with earthworms (*Eisenia fetida*) in artificial soil (5.2% organic matter) according to OECD TG 222 is mentioned. Five exposure concentrations were used, varying from 250 to 4000 mg/kg dw with a spacing factor of 2. Adverse effects were observed for both the adult worms as the number of juveniles. The NOECs and EC10s were 2000 and 3264 mg/kg dw for mortality and 250 and 543 mg/kg dw for body mass change of adult earthworms after 28 days, and 500 and 724 mg/kg dw for reproduction (number of juveniles) after 56 days.

In the registration dossier for TPPT these NOECs have been expressed on the content of TPPT, assuming as worst-case that all toxicity can be attributed to TPPT. The reported EC10s were 900 mg/kg dry weight soil for mortality of adult earthworms after 28 days and 199.6 mg/kg dw for reproduction (number of juveniles) after 56 days.

5.2.2 Toxicity to terrestrial plants

No relevant information available.

5.2.3 Toxicity to soil micro-organisms

In the registration dossier of the reaction mass of: triphenylthiophosphate and *tert*-butylated derivatives, also a toxicity test to soil microorganisms according to OECD TG 216 with this substance from 2017 is mentioned, showing no adverse effects. No further information is given in this dossier.

In the registration of TPPT some more information is given. Five exposure concentrations were used, varying from 62.5 to 1000 mg/kg dw with a spacing factor of 2. Nitrate formation was measured after 0, 7, 14, and 28 days. No inhibitory effects were observed. Therefore, the EC10 is reported to be >1000 mg/kg dw test substance or >275.7 mg/kg dw expressed as TPPT.

5.2.4 Toxicity to other terrestrial organisms

No relevant information available.

5.3 Atmospheric compartment

No relevant information available.

5.4 Microbiological activity in sewage treatment systems

In the registration dossier of TPPT two inhibition tests according to OECD TG 209 are mentioned. The first study from 1988 is performed with TPPT at a nominal concentration of 100 mg/L. The initial microbial biomass in the test was 1.7 g/L. No inhibitory effects were observed and it is concluded that the NOEC should at least be 100 mg/L.

Another test from 1997 was performed with reaction mass of: triphenylthiophosphate and *tert*-butylated derivatives (EC 421-820-9). Five nominal concentrations were tested, ranging from 10 to 1000 mg/L. The microbial biomass was 0.88 g/L (200 ml of a 2.2 g/L suspension in 500 ml). The NOEC was 320 mg/L test material and the EC20 403 mg/L. Inhibition at the highest concentration of 1000 mg/L was 29.7%.

5.5 Toxicity to birds

No relevant information available.

5.6 Mammalian wildlife

No relevant information available.

5.7 Endocrine disruption (Environment)

Not evaluated

5.8 Other effects

Not evaluated

5.9 Summary and discussion of the environmental hazard assessment

The most sensitive species tested for TPPT was the rainbow trout (*Oncorhynchus mykiss*) with a chronic EC10 of 2.2 ug/L derived from a very good dose response curve for mortality. The NOEC was considered to be 1.7 ug/L although a statistically significant reduction in survival (95%) was already observed at this concentration.

6. Conclusions on the SVHC Properties

6.1 CMR assessment

Not relevant for the identification of the substance as SVHC in accordance with Article 57 (d) of the REACH Regulation.

6.2 PBT and vPvB assessment

6.2.1 Assessment of PBT/vPvB properties

A weight-of-evidence determination according to the provisions of Annex XIII of REACH is used to identify the substance O,O,O-triphenyl phosphorothioate (TPPT) as a PBT substance. All available information (such as the results of standard tests and modelling, analogue approach (read-across) and (Q)SAR results) was considered together in a weight-of-evidence approach. As reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives contains more than 0.1% TPPT, this substance can also be identified as a PBT substance.

6.2.1.1 Persistence

QSAR predictions on biodegradation indicate borderline persistence. Reliable screening tests of ready biodegradability according to OECD TG 301B, C and D with either TPPT or reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9) show that TPPT is not readily biodegradable with mineralisation generally below 20% after 28 days. In the simulation test with natural pond water, according to OECD TG 309, there was no indication of any significant degradation over the test duration of 61 days. Further, a hydrolysis test showed that primary degradation by abiotic hydrolysis is slow with an extrapolated aqueous half-life of 278 days at pH 7 and 12 °C. The outcome of the simulation test in water together with the results of the screening tests and the hydrolysis test, leads to the conclusion that TPPT is very persistent (vP), well exceeding the fresh water half-life criterion of 60 days for vP.

6.2.1.2 Bioaccumulation

The bioaccumulation study performed with carp exposed to reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9) shows bioconcentration factors for TPPT close to or exceeding 2000, based on the low exposure test concentration which is the reliable part of the study (Klimisch 2) . Normalised to 5% lipids, kinetic BCF_{KL}s based on the data from the uptake phase are in excess of 2000 (2112 L/kg for the lower tested concentration). When accounting for the reduced bioavailability, due to the application of TPPT in a mixture, the BCF values for TPPT would turn out even higher. These data together are considered sufficient to conclude that TPPT at least meets the B criterion (BCF > 2000).

6.2.1.3 Toxicity

An early life stage (ELS)-test with rainbow trout resulted in a NOEC for TPPT of 1.7 µg/L, which is below the toxicity criterion of 10 µg/L. This study confirmed that the toxicity observed for fish in a toxicity test with the reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives, can be attributed to TPPT with a NOEC below the T criterion of 10 µg/L. It can thus be concluded that TPPT meets the T-criterion.

6.2.2 Summary and overall conclusions on the PBT and vPvB properties

A weight-of-evidence determination according to the provisions of Annex XIII of REACH is used to identify the substance O,O,O-triphenyl phosphorothioate (TPPT) as a PBT substance. All available information (such as the results of standard tests and modelling, analogue approach (read-across) and (Q)SAR results) was considered together in a weight-of-evidence approach. As Reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives contains more than 0.1% TPPT, this substance can also be identified as a PBT substance.

Persistence

QSARs predictions on biodegradation indicate borderline persistence. Reliable screening tests of ready biodegradability according to OECD TG 301B, C and D with either TPPT or Reaction mass of: triphenylthiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9) show that TPPT is not readily biodegradable with mineralisation generally below 20% after 28 days. The ready biodegradability studies are given a medium weight in the weight of evidence assessment.

In a reliable simulation test with natural pond water, performed on TPPT according to OECD TG 309, there was no indication of any significant degradation over the test duration of 61 days, while the reference substance showed high mineralisation in 14 days. It can thus be concluded that the half-life in fresh surface water is >>61 days. The simulation test is given a high weight in the weight of evidence assessment.

Further, a hydrolysis test according to OECD TG 111 performed on TPPT showed that primary degradation by abiotic hydrolysis is slow with an extrapolated aqueous half-life of 278 days at pH 7 and 12 °C.

The outcome of the simulation test in water together with the results of the screening tests and the hydrolysis test, leads to the conclusion that TPPT meets the 'persistence' criterion (P) and the 'very persistent' criterion (vP) in accordance with Annex XIII, points 1.1.1 and 1.2.1, of the REACH Regulation on the basis of its persistent and very persistent (P/vP) properties in fresh water (degradation half-lives > 60 days).

Bioaccumulation

The screening criteria for bioaccumulation in aquatic organisms (log K_{ow} > 4.5) is fulfilled for TPPT based on the measured log K_{ow} value of 5.0 estimated by the HPLC method (OECD TG 117).

A bioaccumulation study performed with carp exposed to Reaction mass of: triphenyl thiophosphate (TPPT) and tertiary butylated phenyl derivatives (EC 421-820-9) shows bioconcentration factors for TPPT close to or exceeding 2000, based on the low exposure test concentration which is the reliable part of the study (Klimisch 2). Normalised to 5% lipids, kinetic BCF_{KL}s based on the data from the uptake phase are in excess of 2000 (2112 L/kg for the lower tested concentration). When accounting for the reduced bioavailability, due to the application of TPPT in a mixture, the BCF values for TPPT would turn out even higher. The study was conducted to GLP following the Japanese test guideline "Bioaccumulation test of a chemical substance in fish or shellfish" provided in "the Notice on the Test Method Concerning New Chemical Substances" and is considered to be reliable with restrictions. The fish bioaccumulation test is given a high weight in the weight of evidence assessment.

The outcome of the fish bioaccumulation test together with the fact that the measured log K_{ow} of TPPT is >4.5 leads to the conclusion that TPPT meets the 'bioaccumulative' criterion (B) in accordance with Annex XIII, point 1.1.2 of the REACH Regulation on the basis of its bioaccumulative properties in fish (fish BCF > 2000).

Toxicity

A fish early life stage test according to OECD TG 210 performed on TPPT with rainbow trout under flow-through conditions resulted in a larval survival NOEC for TPPT of 1.7 µg/L, which is below the toxicity criterion of 10 µg/L. This test is reliable and is given a high weight in the weight of evidence assessment.

A toxicity test with Reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9) was performed on rainbow trout according to OECD TG 210. Although the dose-response modelling is hampered by the steep-dose response, it is clear that the EC10s are between the concentrations of 8.7 and 17 µg/L. If the toxicity of the mixture would be fully attributed to TPPT, the EC10 for larval survival would be 4.2 µg/L, i.e. slightly higher than observed in the test with pure TPPT. This test reliable with restrictions and is given a high weight in the weight of evidence assessment.

The results of the fish early life stage tests lead to the conclusion that TPPT meets the ‘toxicity’ criterion (T) in accordance with Annex XIII, point 1.1.3 of the REACH Regulation on the basis of its toxic properties to fish (fish NOEC < 10 µg/L).

Conclusion

TPPT is very persistent. In a simulation test in water according to OECD TG 309 there was no significant degradation of the substance over a period of 61 days, resulting in a half-life >>60 d and thus fulfilling the P and vP criteria.

TPPT is bioaccumulative. In a bioconcentration test with carp exposed to reaction mass of: triphenyl thiophosphate and tertiary butylated phenyl derivatives (EC 421-820-9), the kinetic BCF of TPPT normalised to 5% lipids exceeds the B criterion of 2000 L/kg, based on the low exposure test concentration which is the reliable part of the study (Klimisch 2).

TPPT is toxic. The NOEC for TPPT in a fish early life-stage test with rainbow trout was 1.7 µg/L for mortality, which is well below the T criterion of 10 µg/L.

In conclusion, TPPT can be identified as a PBT substance according to Art. 57(d) of REACH by comparing all relevant and available information listed in Annex XIII of REACH with the criteria set out in the same Annex, in a weight-of-evidence determination.

As reaction mass of: triphenylthiophosphate and its tert-butylated phenyl derivatives (EC 421-820-9) contains more than 0.1% TPPT, this substance can also be identified as a PBT substance according to Art. 57(d) of REACH.

6.3 Assessment under Article 57(f)

This section is not relevant for the identification of the substance as SVHC in accordance with Article 57 (d) of the REACH Regulation.

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