SUBSTANCE EVALUATION REPORT

Public Name: Reaction products of 4-methyl-2-pentanol and diphosphorus pentasulfide, propoxylated, esterified with diphosphorous pentaoxide, and salted by amines, C12-14- tert—alkyl (former name: Reaction products of bis(4-methylpentan-2-yl)dithiophosphoric acid with phosphorus oxide, propylene oxide and amines, C12-14-alkyl (branched))

EC Number(s): 931-384-6

CAS Number(s):/

Submitting Member State Competent Authority: Chemicals Office of the R Slovenia, Ajdovščina 4, 1000 Ljubljana, Slovenia

Year of evaluation: 2013

VERSION NUMBER: [3] **DATE: [**20 October 2014**]**

Conclusions of the most recent evaluation step*	Tick relevant box(es)
Concern not clarified; Need to request further information from the Registrant(s) with the draft decision	
Concern clarified; No need of further risk management measures	X
Concern clarified; Need for risk management measures; RMO analysis to be performed	
Other: [*please specify*]	

DISCLAIMER

The report has been prepared by the evaluating Member State as a part of the substance evaluation process under the REACH Regulation (EC) No 1907/2006. The information and views set out in this document are those of the author and do not necessarily reflect the position or opinion of the European Chemicals Agency or other Member States. The Agency does not guarantee the accuracy of the information included in the report. Neither the Agency nor the evaluating Member State nor any person acting on either of their behalves may be held liable for the use which may be made of the information contained therein. Statements made or information contained in the report are without prejudice to any further regulatory work that the Agency or Member States may initiate at a later stage.

Executive summary

Grounds for concern

The initial grounds for concerns from the justification document in the CoRAP 2013 were a suspected PBT/vPvB and there was consumer use in lubricants and greases. Due to the fact that the molecular formula of this organic UVCB substance is not specified and the fact that substance is a complex reaction mixture with variable composition which leads to difficulties in substance identification and wide variation in given phys-chem parameters the identity of the substance was identified as a concern as well.

Substance has a low vapour pressure (0.032 Pa at 25 °C).
Water solubility is reported to be loading dependent

- 39.5 mg/L at loading rate 100 mg/L
- 138 mg/L at loading rate 1000 mg/L

Partitioning coefficient log Pow ranges from < 0.3 to > 7.10 (OECD 117) of which 59% between log Pow 1.81- 6.
Reported Log Koc values ranged from < 1.25 to 5.09 (EU Method C.19 but outside the calibration standards)
Distribution within STP (EUSES 2.1) indicates partitioning to water (13.1%) and sludge (86.9%).

Persistency
Degradation of the registered substance was very low after 28 days in several ready biodegradation tests with adapted inoculum.

- 3.6 % (28 days) ASTM D-5864-95 (standard test method for determining aerobic aquatic biodegradation of lubricants or their components)
- From -10 % to 7.4 % (28 days) OECD 301B Pre-exposed inoculum.

Screening criteria for persistence are met. There is a possible inhibition of the inoculum in the ready biodegradability tests (negative biodegradation values). No hydrolysis or photo transformation data available. Simulation tests are waived.
Substance is potentially P/vP.

Bioaccumulation
Molecular weight of the registered substance varies between Mw 181.1-773.3 that indicates potential for bioaccumulation. In addition, there is high variability in log Pow (< 0.3 (3 %), 1.81 – 6 (59%), > 7.1 (38%)) also indicating potential for bioaccumulation.

Reported BCF (EPA OPPTS 850.1730) is based on read across (S-2-hydroxypropyl O,O-bis(4-methylpentan-2yl) phosphorodithioate, and Dithiophosphoric acid O,O'-bis-(1,3-dimethyl-butyl) ester S-(2-hydroxy-propyl) ester); BCF at the low exposure level was 426 and BCF in the high exposure level was 432. Representativeness of the read across to predict bioaccumulation of registered UVCB is unclear.

Report on BCFWIN and Gobas models were used to predict bioaccumulation of two types of phosphate esters, sulphur and non-sulphur containing substances (11 substances). Report concluded that BCF does not exceed 5,000 l/kg ww; i.e. the vB criterion. However, no clear interpretation on BCF in relation to the registered substance was given.

Toxicity
All ecotoxicity testing is based on water accumulated fraction (WAF) approach.
Definitive criteria were not met but there was clear indication for potential toxicity. Using nominal concentrations does not give a realistic picture of the toxicity of the substance.

Long term Daphnia (OECD 211); NOEC 0.12 mg/L (WAF max 12 mg/L), EL50 0.66 mg/L

OECD 201 Algae (WAF max 25 mg/L); NOEC 1.7 mg/L, EC50 6.4 mg/L
OECD 202 Daphnia; read across EC 294-716-2 (Amines, C12-14-alkyl, reaction products with hexanol, phosphorus oxide (P2O5), phosphorus sulfide (P2S5) and propylene oxide) (WAF max 99.5 mg/L =TOC 5 ppm), EC50 91 mg/L
OECD 203 Fish; (WAF) LL50 24 mg/l, NOELR 3.2 mg/L (max loading 32 mg/L), sublethal effects were observed at 5.6 mg/L (WAF)

The substance is potentially PB(T). Evaluation of T depends on the approach taken with WAF concentrations. Registrant suggests that the substance is potentially P but not B or T.

The substance evaluation shall clarify the following issues:
- UVCB substance identity
- Simulation test on biodegradability in soil
- Read across approach on bioaccumulation studies
- Using WAF concentration in T assessment leads to uncertainty

Procedure

The substance evaluation is based on information in the aggregated registration dossier (technical dossier, IUCLID), the Chemical Safety Report (CSR) but also other relevant literature and regulatory information were assessed. During the evaluation the representative of the Registrants has been contacted by the Slovene competent authority (CA) in order to discuss initial concerns. All updates received until 12/2013 were considered. The evaluation is also complemented with information provided by relevant studies mostly conducted in the 90's and after the year 2000 with the latest ones originating from 2009 but there is some literature from the 80's or earlier years as well.
The evaluation as well as the documentation in the substance evaluation report focuses on the initial concerns. The evaluation was targeted on:
1. Information related to the (UVCB) substance identity
2. Information related to the PBT assessment:

The Slovene CA concluded that it is not necessary to request new data and therefore a draft decision is not prepared. In addition the substance evaluation can be concluded with a report, based upon the following conclusions.

Conclusions

It is recommended that the substance is named **Reaction products of 4-methyl-2-pentanol and diphosphorus pentasulfide, propoxylated, esterified with diphosphorous pentaoxide, and salted by amines, C12-14- tert—alkyl**.

The further clarification on the identity of the substance is considered adequate for an UVCB substance. Analysing the exact composition is hampered by the formation of multi-component complexes but qualitative identification of the constituents is adequate.

The substance under evaluation is not considered a PBT or vPvB substance, since none of the constituents fulfils endpoint criteria for B or vB.

Based on the conclusions of the substance evaluation (SEV) no further risk management measures are needed.

Statement of reasons

Not applicable, as a draft decision was not prepared.

CONTENTS

1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

1.1 Name and other identifiers of the substance

The registrant submitted further information on the identity of the substance in December 2013 (Conf.ref.1, 2013a). The substance under evaluation was originally described as **Reaction products of bis(4-methylpentan-2-yldithiophosphoric acid with phosphorus oxide, propylene oxide and amines, C12-14-alkyl (branched)**. Based on a SID CCH decision of ECHA[1], which is publically available, the name of evaluated substances has changed to Reaction products of 4-methyl-2-pentanol and diphosphorus pentasulfide, propoxylated, esterified with diphosphorous pentaoxide, and salted by amines, C12-14- tert—alkyl and further information was provided on the identity of the substance.

The registrant identified unsalted amine, unreacted alcohol, and polypropylene as impurities. It is noted that due to the lack of differentiation between constituents and impurities, the term “main constituents” and “impurities” should not be regarded as relevant for UVCB substances.

Analysis of EC No. 931-384-6 was also conducted by HPLC utilizing ESI-MS to assist in the determination of the composition of each of the fractions isolated (Conf.ref.3, 2003). Initial review of the chromatogram indicated that it was possible to separate the product into different fractions. Each of the isolated fractions was subjected to Electrospray Ionization mass spectrometry (ESI-MS), which was utilized to analyze the chemical composition of the HPLC fractions. ESI-MS was utilized as it generally provides molecular ions with little to no fragmentation. The absence of significant fragmentation is important in the identification of components of a complex reaction mixture. In order to be able to compare the fractions, a sample of EC No. 931-384-6 was also analyzed by ESI-MS. Most of the significant ions observed in these spectra are from known major components of the substance.

ESI-MS of the EC No. 931-384-6 cannot be used for quantification. This product contains a number of very different chemical species of widely varying molecular weight, and so detection efficiency is expected to be variable. Since it is not technically feasible to separate the individual components, it is not possible to determine their individual detection efficiency. Thus the ESI-MS data can be used for determining what is present, but not for quantifying individual species.

Based on the available information, the substance is still identified as an UVCB substance, because the ratio between constituents is variable and poorly predictable. Analysing the exact composition is hampered by the formation of multi-component complexes, but otherwise constituents can be qualitatively identified.

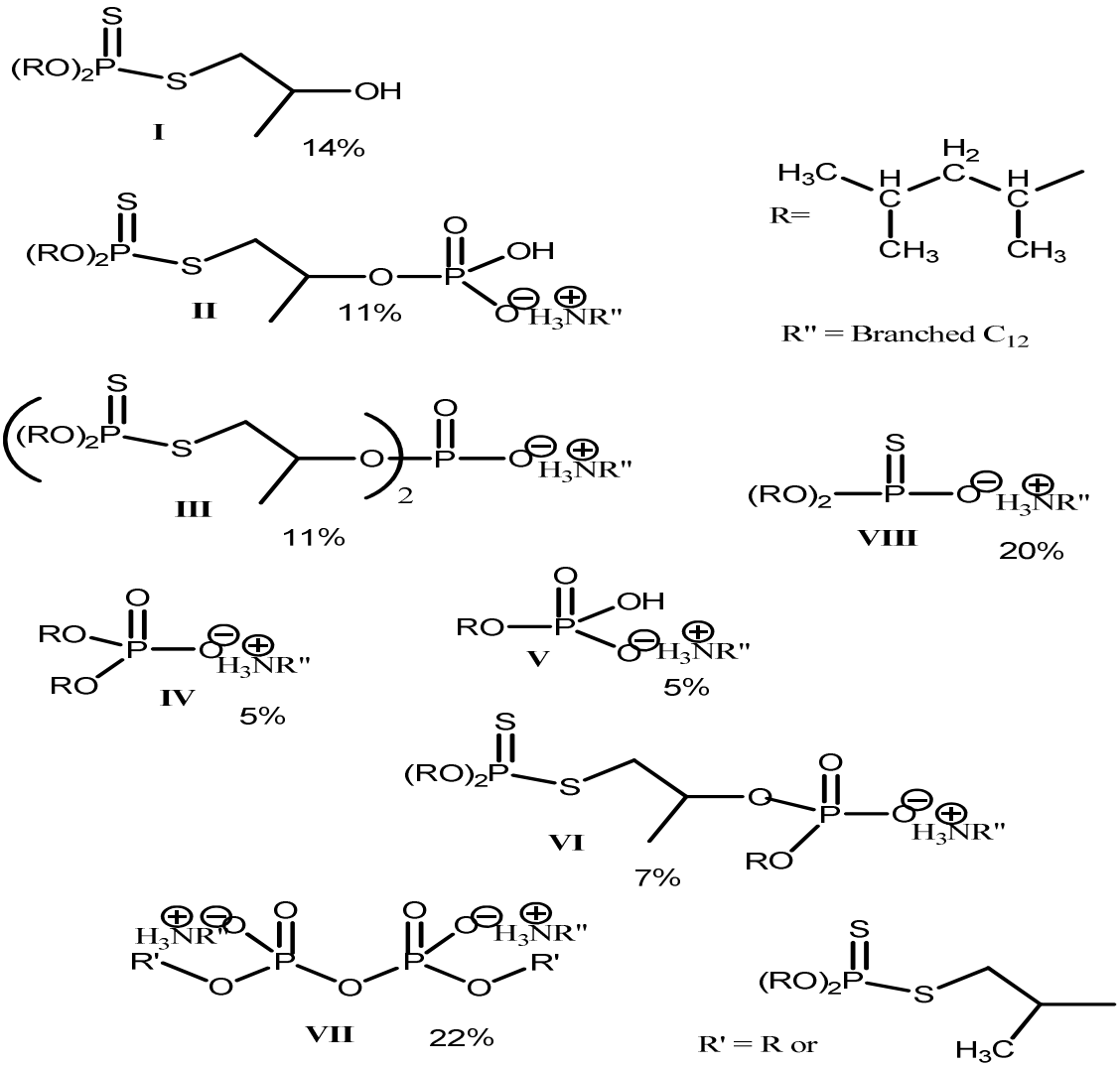
Some of the representative molecular structures contain one or more chiral centres. While two of the starting materials utilized contain chiral centres (4-methyl-2-pentanol and propylene oxide), only the racemic versions of these materials are utilized. There are no chiral catalysts utilized in the production that would influence the chirality of the product produced. Therefore the material characterized by EC No. 931-384-6 is racemic (Conf.ref.2, 2013b).

[1] http://echa.europa.eu/regulations/reach/evaluation/requests-for-further-information/evaluation-decisions

Table 1: Substance identity

Public Name:	Reaction products of 4-methyl-2-pentanol and diphosphorus pentasulfide, propoxylated, esterified with diphosphorous pentaoxide, and salted by amines, C12-14- tert-alkyl
EC number:	931-384-6
EC name:	/
CAS number (in the EC inventory):	/
CAS number:	/
CAS name:	/
IUPAC name:	Reaction products of 4-methyl-2-pentanol and diphosphorus pentasulfide, propoxylated, esterified with diphosphorus pentaoxide, and salted by amines, C12-14- tert-alkyl
Index number in Annex VI of the CLP Regulation	/
Molecular formula:	Too complex
Molecular weight range:	181.1-773.3
Synonyms:	/

Structural formula: The substance is a UVCB. Representative structures are presented below:



1.2 Composition of the substance

Name: Reaction products of 4-methyl-2-pentanol and diphosphorus pentasulfide, propoxylated, esterified with diphosphorous pentaoxide, and salted by amines, C12-14- tert—alkyl

Description: UVCB

Degree of purity: Not relevant

Data (table) on constituents provided in Chemical Safety Report are included in Annex: Confidential information.

Table 2: Impurities

Impurities	Typical concentration	Concentration range	Remarks
/	/	/	/

Table 3: Additives

Additives	**Typical concentration**	**Concentration range**	**Remarks**
/	/	/	/

1.3 Physico-chemical properties

Table 4 : Overview of physicochemical properties

Property	Value	Remarks
Physical state at 20°C and 101.3 kPa	Liquid Form: viscous Colour: amber Odour: characteristic of sulfur-containing compounds	
Melting/freezing point	pour point: - 6 ^{o}C	
Boiling point	The test material's weight loss associated with decomposition occurred at temperatures of 209, 250 and 529 ^{o}C. The onset of decomposition occurred at 198 ^{o}C.	
Relative density	1.02 at 15.6 ^{o}C	
Vapour pressure	0.032 Pa at 25 ^{o}C	
Surface tension	Based on the known chemical composition, surface activity is not expected.	In accordance with REACH Regulation, Annex VII, section 7.6, column 2, the study was not conducted. Based on the known chemical composition, surface activity is not expected.
Water solubility	The water solubility of the test material is loading rate dependent: 39.5 mg/L (at loading rate 100 mg/L) and 138 mg/L (at loading rate 1000 mg/L).	
Partition coefficient n-octanol/water (log value)	Log Pow ranges from < 0.30 to >7.10.	
Flash point	Range 61.0 – 78.73°C at 760 mm Hg	
Flammability	Not pyrophoric, not flammable on contact with water.	Testing for this endpoint is waived based on a consideration of the chemical structure and experience in handling and use.
Explosive properties	Not explosive.	The study is waived because no structural alert for explosiveness, and based on long-term experience with handling and use of the substance.

Property	Value	Remarks
Oxidising properties	Not oxidising.	The study is waived because the substance is incapable of reacting exothermically with combustible materials; also based on the long-term experience with handling and use of the substance.
Granulometry	Not applicable. The substance is marketed or used in liquid form.	
Stability in organic solvents and identity of relevant degradation products	Formulation of test material in Arachis Oil BP was stable for at least 4h.	Information extract from the Reproduction/ Developmental Toxicity Screening test.
Dissociation constant	No data available	The study is waived because study is technically not feasible.
Viscosity	46.827 cSt at 100 ^{o}C	
Auto flammability	The auto-ignition temperature of the test substance is 286 ^{o}C at 102.09 kPa.	
Reactivity towards container material		Data not required for this tonnage.
Thermal stability		Data not required for this tonnage.

2 MANUFACTURE AND USES

2.1 Quantities

Data (table) on aggregated tonnage (per year) provided in Chemical Safety Report are included in Annex: Confidential information.

2.1.1 Manufacturing processes

Manufacture of the test material is not relevant and not covered in this report.

2.2 Identified uses

2.2.1 Uses by workers in industrial settings

Table 5: Uses by workers in industrial settings

IU No.	Identified Use (IU) name	Substance supplied to that use	Use descriptors
1	Industrial formulation of lubricant additives, lubricants and greases	in a mixture	**Process category (PROC):** PROC 1: Use in closed process, no likelihood of exposure PROC 2: Use in closed, continuous process with occasional controlled exposure PROC 3: Use in closed batch process (synthesis or formulation) PROC 4: Use in batch and other process (synthesis) where opportunity for exposure arises PROC 5: Mixing or blending in batch processes for formulation of preparations and articles (multistage and/or significant contact) PROC 8a: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities PROC 8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities PROC 9: Transfer of substance or preparation into small containers (dedicated filling line, including weighing) PROC 15: Use as laboratory reagent **Environmental release category (ERC):** ERC 2: Formulation of preparations **Sector of end use (SU):** SU 10: Formulation [mixing] of preparations and/or re-packaging (excluding alloys) **Subsequent service life relevant for that use?:** no

IU No.	Identified Use (IU) name	Substance supplied to that use	Use descriptors
2	Industrial formulation of lubricant additives, lubricants and greases	in a mixture	**Process category (PROC):** PROC 1: Use in closed process, no likelihood of exposure PROC 2: Use in closed, continuous process with occasional controlled exposure PROC 8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities PROC 9: Transfer of substance or preparation into small containers (dedicated filling line, including weighing) **Environmental release category (ERC):** ERC 4: Industrial use of processing aids in processes and products, not becoming part of articles ERC 7: Industrial use of substances in closed systems **Sector of end use (SU):** SU 0: Other: SU3: Industrial uses: Uses of substances as such or in preparations* at industrial sites **Subsequent service life relevant for that use?:** no
3	Industrial use in open system: application of lubricant to work pieces or equipment by dipping, brushing or spraying (without exposure to heat).	in a mixture	**Process category (PROC):** PROC 7: Industrial spraying PROC 8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities PROC 9: Transfer of substance or preparation into small containers (dedicated filling line, including weighing) PROC 10: Roller application or brushing PROC 13: Treatment of articles by dipping and pouring **Environmental release category (ERC):** ERC 4: Industrial use of processing aids in processes and products, not becoming part of articles **Sector of end use (SU):** SU 0: Other: SU3: **Subsequent service life relevant for that use?:** no

2.2.2 Use by professional workers

Table 6: Use by professional workers

IU number	Identified Use (IU) name	Substance supplied to that use	Use descriptors
4	Professional use of lubricants and greases in vehicles or machinery	in a mixture	**Process category (PROC):** PROC 1: Use in closed process, no likelihood of exposure PROC 2: Use in closed, continuous process with occasional controlled exposure PROC 8a: Transfer of substance or

IU number	Identified Use (IU) name	Substance supplied to that use	Use descriptors
			preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities PROC 8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities PROC 20: Heat and pressure transfer fluids in dispersive, professional use but closed systems **Environmental release category (ERC):** ERC 9a: Wide dispersive indoor use of substances in closed systems ERC 9b: Wide dispersive outdoor use of substances in closed systems **Sector of end use (SU):** **Subsequent service life relevant for that use?:** yes
5	Professional use in open system: application of lubricant to work pieces or equipment by dipping, brushing or spraying (without exposure to heat).	in a mixture	**Process category (PROC):** PROC 1: Use in closed process, no likelihood of exposure PROC 2: Use in closed, continuous process with occasional controlled exposure PROC 8a: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities PROC 10: Roller application or brushing PROC 11: Non industrial spraying **Environmental release category (ERC):** ERC 8a: Wide dispersive indoor use of processing aids in open systems ERC 8d: Wide dispersive outdoor use of processing aids in open systems **Sector of end use (SU):** **Subsequent service life relevant for that use?:** no

2.2.3 Uses by consumers

Table 7: Uses by consumers

IU number	Identified Use (IU) name	Substance supplied to that use	Use descriptors
4	Professional use of lubricants and greases in	in a mixture	**Process category (PROC):** PROC 1: Use in closed process, no

IU number	Identified Use (IU) name	Substance supplied to that use	Use descriptors
	vehicles or machinery		likelihood of exposure PROC 2: Use in closed, continuous process with occasional controlled exposure PROC 8a: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities PROC 8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities PROC 20: Heat and pressure transfer fluids in dispersive, professional use but closed systems **Environmental release category (ERC):** ERC 9a: Wide dispersive indoor use of substances in closed systems ERC 9b: Wide dispersive outdoor use of substances in closed systems **Sector of end use (SU):** **Subsequent service life relevant for that use?:** yes
5	Professional use in open system: application of lubricant to work pieces or equipment by dipping, brushing or spraying (without exposure to heat).	in a mixture	**Process category (PROC):** PROC 1: Use in closed process, no likelihood of exposure PROC 2: Use in closed, continuous process with occasional controlled exposure PROC 8a: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities PROC 10: Roller application or brushing PROC 11: Non industrial spraying **Environmental release category (ERC):** ERC 8a: Wide dispersive indoor use of processing aids in open systems ERC 8d: Wide dispersive outdoor use of processing aids in open systems **Sector of end use (SU):** **Subsequent service life relevant for that use?:** no

2.3 Uses advised against

None.

2.3.1 Uses by workers in industrial settings advised against

None.

2.3.2 Use by professional workers advised against

None.

2.3.3 Uses by consumers advised against

None.

3 CLASSIFICATION AND LABELLING

3.1 Harmonised Classification in Annex VI of the CLP Regulation

Substance has not yet been included in Annex VI of the CLP Regulation (EC) No 1272/2008.

3.2 Self classification

Self-classification reported by the registrant is as follows:

- For physical-chemical properties:

Endpoints	Classification / Reason for no classification
Explosives:	Reason for no classification: conclusive but not sufficient for classification
Flammable gases:	Reason for no classification: data lacking
Flammable aerosols:	Reason for no classification: data lacking
Oxidising gases:	Reason for no classification: data lacking
Gases under pressure:	Reason for no classification: data lacking
Flammable liquids:	Reason for no classification: conclusive but not sufficient for classification
Flammable solids:	Reason for no classification: data lacking
Self-reacting substances and mixtures:	Reason for no classification: conclusive but not sufficient for classification
Pyrophoric liquids:	Reason for no classification: conclusive but not sufficient for classification
Pyrophoric solids:	Reason for no classification: data lacking
Self-heating substances and mixtures:	Reason for no classification: data lacking
Substances and mixtures which in contact with water emits flammable gases:	Reason for no classification: conclusive but not sufficient for classification
Oxidising liquids:	Reason for no classification: conclusive but not sufficient for classification

Oxidising solids:	Reason for no classification: data lacking
Organic peroxides:	Reason for no classification: data lacking
Corrosive to metals:	Reason for no classification: data lacking

- **For health hazards:**

Endpoints	**Classification / Reason for no classification**
Acute toxicity - oral:	Acute Tox. 4 (Hazard statement: H302: Harmful if swallowed.)
Acute toxicity - dermal:	Reason for no classification: data lacking
Acute toxicity - inhalation:	Reason for no classification: data lacking
Skin corrosion/irritation:	Reason for no classification: conclusive but not sufficient for classification
Serious damage/eye irritation:	Eye Damage 1 (Hazard statement: H318: Causes serious eye damage.)
Respiration sensitization:	Reason for no classification: data lacking
Skin sensitation:	Skin Sens. 1 (Hazard statement: H317: May cause an allergic skin reaction.)
Aspiration hazard:	Reason for no classification: conclusive but not sufficient for classification
Reproductive Toxicity:	Reason for no classification: conclusive but not sufficient for classification
Reproductive Toxicity: Effects on or via lactation:	Reason for no classification: data lacking
Germ cell mutagenicity:	Reason for no classification: conclusive but not sufficient for classification
Carcinogenicity:	Reason for no classification: data lacking
Specific target organ toxicity - single:	Reason for no classification: conclusive but not sufficient for classification
Specific target organ toxicity - repeated:	Reason for no classification: conclusive but not sufficient for classification

Specific concentration limits for health hazard:

Concentration (%)	**Classification**
> 50.0 <= 100.0	Eye Damage 1

- **For environmental hazards:**

Endpoints	**Classification / Reason for no classification**
Hazards to the aquatic environment:	Aquatic Chronic 2 (Hazard statement: H411: Toxic to aquatic life with long lasting effects.)

Labelling

Signal word: Warning

Hazard pictogram:

GHS07: exclamation mark

GHS09: environment

Hazard statements:

H302: Harmful if swallowed.
H317: May cause an allergic skin reaction.
H318: Causes serious eye damage.
H411: Toxic to aquatic life with long lasting effects.

Precautionary statements:

P280: Wear protective gloves/protective clothing/eye protection/face protection.
P305+P351+P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310: Immediately call a POISON CENTER or doctor/physician.
P261: Avoid breathing dust/fume/gas/mist/vapours/spray.
P273: Avoid release to the environment.
P363: Wash contaminated clothing before reuse.
P333+P313: If skin irritation or rash occurs: Get medical advice/attention.
P391: Collect spillage.
P302+P352: IF ON SKIN: Wash with plenty of soap and water.
P501: Dispose of contents/container to...

4 ENVIRONMENTAL FATE PROPERTIES

4.1 Degradation

4.1.1 Abiotic degradation

4.1.1.1 Hydrolysis

Data on hydrolysis are not available for the substance. Justification provided in Chemical Safety Report is following: in accordance with Annex XI, the study does not need to be conducted if it is not scientifically possible to perform the test due to the properties of the test substance or because of analytical limitations of the test method. The test material is an incompletely characterized material (UVCB) consisting of a mixture of components with multiple functional groups that form complexes which it has not been possible to separate by chromatographic methods. Spectrometric methods such as IR detect functional groups but not individual components; mass spectrometry generates fragment ions rather than intact molecular ions. Additionally, the water solubility of this substance has been determined to be loading rate dependent and the composition of the substance in water might vary depending on loading. The lack of specificity of spectrometric methods and the lack of resolution by chromatographic methods limits our ability to detect or identify changes in this substance that can conclusively be attributed to hydrolysis**.**

4.1.1.2 Phototransformation/photolysis

4.1.1.2.1 Phototransformation in air

Data on phototransformation in air are not available for the substance

4.1.1.2.2 Phototransformation in water

Data on phototransformation in air are not available for the substance

4.1.1.2.3 Phototransformation in soil

Data on phototransformation in air are not available for the substance

4.1.2 Biodegradation

4.1.2.1 Biodegradation in water

4.1.2.1.1 Estimated data

Estimated data are not available for the substance.

4.1.2.1.2 Screening tests

It can be concluded that screening criteria for persistence are met. There is possible inhibition of the inoculum in the ready biodegradability tests (negative biodegradation values).

Table 8: An overview of screening tests for biodegradation in water

Method	Results	Remarks	Reference
Test type: ready biodegradability activated sludge, domestic, adapted ASTM D-5864-95	Under test conditions no biodegradation observed % Degradation of test substance: 3.6 after 28 d (CO_2 evolution)	1 (reliable without restriction) key study experimental result Test material (IUPAC name): Reaction products of bis(4-methylpentan-2-yl)dithiophosphoric acid with phosphorus oxide, propylene oxide and amines, C12-14-alkyl (branched)	Schaefer, E. C., Siddiqui, A. I. (2003)
Test type: ready biodegradability activated sludge, domestic, adapted OECD Guideline 301 B (Ready Biodegradability: CO_2 Evolution Test)	under test conditions no biodegradation observed % Degradation of test substance: -10 after 28 d (CO_2 evolution) (Negative values for %degradation.)	1 (reliable without restriction) supporting study experimental result **Test material (IUPAC name): Reaction products of bis(4-methylpentan-2-yl)dithiophosphoric acid with phosphorus oxide, propylene oxide and amines, C12-14-alkyl (branched)**	Schaefer, E.C., Siddiqui, A.I. (2004)
Test type: ready biodegradability Supernatant from suspended solids passed through a primary clarifier at a wastewater treatment facility OECD Guideline 301 B (Ready Biodegradability: CO_2 Evolution Test)	under test conditions no biodegradation observed % Degradation of test substance: ca. 7.4 after 28 d (CO2 evolution)	2 (reliable with restrictions) supporting study experimental result **Test material (IUPAC name): Reaction products of bis(4-methylpentan-2-yl)dithiophosphoric acid with phosphorus oxide, propylene oxide and amines, C12-14-alkyl (branched)**	Schaefer, E.C., Griefer, B. (1994)
Test type: ready biodegradability mixture of activated sludge and soil OECD Guideline 301 B (Ready Biodegradability: CO_2	under test conditions no biodegradation observed % Degradation of test substance: -4.7 after 28 d (CO_2 evolution) (Test material added to medium by pre-	1 (reliable without restriction) supporting study experimental result **Test material (IUPAC name): Reaction products of bis(4-methylpentan-2-yl)dithiophosphoric acid with**	Schaefer, E.C., Matthews, M. E. (2009)

Method	Results	Remarks	Reference
Evolution Test) EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) equivalent or similar to ISO 10634:1995(E) Water quality - Guidance for the preparation and treatment of poorly water-soluble organic compounds for the subsequent evaluation of their biodegradability in an aqueous medium	application on silica gel) -2.7 after 28 d (CO_2 evolution) (Test material added to test medium by pre-dissolving in silicone oil)	**phosphorus oxide, propylene oxide and amines, C12-14-alkyl (branched)**	

4.1.2.1.3 Simulation tests (water and sediments)

No simulation tests are available for this substance. Justification provided in Chemical Safety Report is following: testing is waived in accordance with Annex IX of REACH Regulation, column 2, sections 9.2.1.2 and 9.2.1.4. The water solubility of the substance is loading rate dependent. At a loading rate of 100 mg/L the substance is only slightly soluble. The direct and indirect exposure of soil is unlikely.

4.1.2.1.4 Summary and discussion of biodegradation in water and sediment

It can be concluded that screening criteria for persistence are met. There is possible inhibition of the inoculum in the ready biodegradability tests (negative biodegradation values).

4.1.2.2 Biodegradation in soil

No data on biodegradation in soil are available for this substance. Justification provided in Chemical Safety Report is included in Annex: Confidential information. Further testing on biodegradation in soil is not considered necessary to conclude on the PBT/vPvB assessment. Based on SEV (substance evaluation) conclusions further testing is not needed (see Section 8.1.4 of this report).

4.1.3 Summary and discussion on degradation

Summary provided in Chemical Safety Report is following: the substance was not readily biodegradable under the conditions of the tests. No experimental testing was possible using Method C7, Abiotic degradation, Hydrolysis as a Function of pH because Method C7 is not suitable for complex mixtures because: a) monitoring of individual components and degradation products would be extremely difficult; and b) the material has been determined to be poorly soluble in water,

and hydrolysis testing would be required at half the saturation concentration value of the component with the lowest water solubility. The NMR profile shows material complexity that makes hydrolysis experiments using standard methods technically not feasible. Data for degradation due to photolysis and in soils and sediments are not available.

Overall, it can be concluded that screening criteria for persistence are met.

4.2 Environmental distribution

4.2.1 Adsorption/desorption

The studies on adsorption/desorption are summarised in the following table:

Table 9: Overview of studies on adsorption/desorption

Method	Results	Remarks	Reference
Study type: adsorption (soil/sewage sludge) HPLC estimation method EU Method C.19 (Estimation of the Adsorption Coefficient (K_{OC}) on Soil and Sewage Sludge Using High Performance Liquid Chromatography (HPLC))	Adsorption coefficient: log Koc: < 1.25 (67.7 area %) log Koc: >= 1.36 <= 5.09 (32.4 area %)	2 (reliable with restrictions) key study experimental result **Test material (IUPAC name): Reaction products of bis(4-methylpentan-2-yl)dithiophosphoric acid with phosphorus oxide, propylene oxide and amines, C12-14-alkyl (branched)**	Walker, J.A., White, D.F. (2009)

4.2.2 Volatilisation

Explanation provided in Chemical Safety Report is following: this substance is not expected to be significantly found in air due to its low vapour pressure. Transport into the atmosphere is not expected to significantly occur due to its low vapour pressure. ECHA guidance classifies substances with vapour pressure values less than 0.1 Pa at 20ºC as very low. (ECHA Guidance R.7, OECD GD 39). Based on vapour pressure of 0.032 Pa at 25ºC this substance is not considered to be a volatile substance is not expected to exist significantly in the vapour phase in the ambient atmosphere (Eisenreich et al. 1981).

4.2.3 Distribution modelling

The following modelling data are available:

Table 10: Overview of distribution modelling

Method	Results	Remarks	Reference
EUSES version 2.1	Partitioning within STP Air: 0.03 % Water: 13.1 % Sludge: 86.9 %	Reliability: 4 The model results are not assignable	EUSES version 2.1

4.2.4 Summary and discussion of environmental distribution

Summary of study results provided in Chemical Safety Report is following: using the data in section above, the partitioning within a sewage treatment plant (STP) has been predicted with EUSES (version 2.1). Significant partitioning to sludge (ca 86.9%) is predicted, with only 13.1% partitioning to water and 0.03% to air.

However it is noted that an overall conclusion on environmental distribution depends on the conclusion of the PBT/vPvB assessment (see also Section 8.1.4 of this report).

4.3 Bioaccumulation

4.3.1 Aquatic bioaccumulation

The studies on aquatic bioaccumulation are summarised in the following table:

Table 11: Overview of studies on aquatic bioaccumulation

Method	Results	Remarks	Reference
Carp (Cyprinus carpio) aqueous (freshwater) flow-through Total uptake duration: 8 wk Details of method: Not applicable equivalent or similar to OECD Guideline 305 (Bioconcentration: Flow-through Fish Test)	436 (whole body d.w.) when tested with 0.25 ug/L test material (measured). 432 (whole body d.w.) when tested with 2.8 ug/L test material (measured). Steady state BCF = mean tissue concentration / mean water concentration Depuration: DT50 ranged from 21 to 28 days depending on the exposure level and tissue type	1 (reliable without restriction) key study experimental result **Test material:** a surrogate molecule of the UVCB substance	Brown, D., Maddock, B.G. (1981)

Explanation provided in Chemical Safety Report is following: extensive BCF modelling conducted by a leading expert in the field of bioaccumulation (Dr. Frank Gobas) confirms the experimental results that bioaccumulation is not likely a significant environmental fate pathway ("Assessment of the Bioconcentration Factors of 11 Compounds in Fish", Frank Gobas, PhD, professor, School of Resource and Environmental Management, Simon Fraser University, November 29, 2005). Several methodologies were used to characterize or estimate the bioconcentration factor of the 11 structures in this material including: searches for empirical bioconcentration, bioaccumulation, and Kow data; estimation of the Kow and Koa; estimation of the degradability; estimation of the BCF using BCFWIN model; estimation of the metabolic transformation rate in fish; and estimation of the BCF using the Gobas models (see References). The expert report by Dr. Frank Gobas also concluded that there is substantial evidence that the substances in this material are not bioaccumulative in fish according to definitions by UNEP LRTAP (United Nations Environment Program Long Range Transboundary Air Pollution) or CEPA (Canadian Environmental Protection Act).

Measured data

A BCF study was conducted on a surrogate molecule of the UVCB substance using rainbow trout based on OPPTS 850.1730 and OECD 305 guideline testing (Wildlife International study completed 2010, entitled "^{14}C-OS242157: A Bioconcentration Test with The Rainbow Trout (Oncorhynchus mykiss))". Because the chemical identity of this substance is very complex, it would not lend itself to conventional tests for bioaccumulation potential. To avoid this situation, a stable molecule with strong similarity to several representative structures of the UVCB substance was synthesized so that reliable bioaccumulation testing could be performed. The surrogate structure is also the predominant constituent of the UVCB product. It is also important to note that the surrogate and representative structure was predicted by QSAR to have a log Kow of around 6.0, a relatively small molecular size (e.g., diameter 10 A), and hence was projected to be lipophilic and potentially bioaccumulative. In the BCF experimental test, a radiolabelled surrogate molecule of 99% purity (see structure below) was tested at two concentrations in water at 0.25 and 2.8 µg/L using a solvent carrier. There was a 35 day uptake period and a 62 day depuration period, during which the fish appeared normal and healthy. Steady state concentrations in the fish tissues were achieved after 31 days. The results from this BCF study in rainbow trout show that this substance had a steady state BCF in whole fish of 436 (not B, not vB) and a kinetic BCF in whole fish of 834 (not B, not vB). These results clearly show that this substance is not bioaccumulative.

Other supporting information

The chemistry of this UVCB substance involves salts of multiple alkyl thiophosphoric acids in an ion pair with the amine salt. The amine (EC#273-279-1; CAS#68955-53-3; "Amines, C12-14-tert-alkyl") is a primary aliphatic amine with highly branched alkyl chains in which the nitrogen atom is linked to a tertiary carbon (C12H28N). Based on EPI Suite modelling and a measured Log Kow value of 2.90 (source: EPA HPV program for CAS#68955-53-3), the 1,1-dimethyldecylammonium component in this substance will have low bioaccumulation potential (i.e., BCF less than 1,000; log Kow less than 4) and does not fulfil the bioaccumulation criterion.

4.3.2 Terrestrial bioaccumulation

No data on terrestrial bioaccumulation are available for this substance. Justification provided in Chemical Safety Report is following: in accordance with REACH legislation the test does not need to be conducted if direct and indirect exposure to the terrestrial compartment is unlikely. In addition, the results of the CSR for this substance and the PEC/PNEC ratios for the local and regional terrestrial compartment indicate no risk. ECHA Chapter R.7B guidance states that if the

PEC/PNEC ratio is below 1, then no risk for the compartment is indicated and there is no need to perform further tests. Furthermore, this substance does not meet the B or vB criterion and it is not considered to be a PBT.

Further testing on terrestrial bioaccumulation is not considered necessary to conclude on PBT (vPvB) assessment (see also Section 8.1.4 of this report).

4.3.3 Summary and discussion of bioaccumulation

The Slovene CA evaluation of the data in relation to the B or vB criterion is presented in Section 8.1.2. Further testing on terrestrial bioaccumulation is not considered necessary to conclude on PBT (vPvB) assessment (see also Section 8.1.4 of this report).

4.4 Secondary poisoning

The Slovene CA evaluation of the data in relation to the B or vB criterion is presented in Section 8.1.2. of this report. Further testing on secondary poisoning is not considered necessary to conclude on PBT (vPvB) assessment (see also Section 8.1.4 of this report).

5 HUMAN HEALTH HAZARD ASSESSMENT

Not evaluated.

6 HUMAN HEALTH HAZARD ASSESSMENT OF PHYSICO CHEMICAL PROPERTIES

Not evaluated.

7 ENVIRONMENTAL HAZARD ASSESSMENT

7.1 Aquatic compartment (including sediment)

7.1.1 Toxicity data

The available aquatic toxicity endpoints are calculated as water-accommodated fraction (WAF) in accordance with the guidance for determining aquatic toxicity of multi-component substances which are only partly soluble in water in OECD (2000)[2], paragraph 3.13. The solubility of the substance was demonstrated to be loading dependent. Determining the toxicity based on WAF (cq. the toxicity for the fraction of multi-component substances that is dissolved and/or present as a

[2] OECD (2000). Guidance document on aquatic toxicity testing of difficult substances and mixtures. OECD Series on Testing and Assessment Number 23, ENV/JM/MONO(2000)6..

stable emulsion in water) is deemed appropriate for the purpose of classification and labelling (see ECHA 2013[3], Section 4.1.4.3) and for PNEC derivation.

However,further testing is not considered necessary to conclude on PBT (vPvB) assessment.

7.1.1.1 Fish

7.1.1.1.1 Short-term toxicity to fish

The results of studies are summarised in the following table::

Table 12 : Overview of short-term effects on fish

Method	Results	Remarks	Reference
Oncorhynchus mykiss freshwater static OECD Guideline 203 (Fish, Acute Toxicity Test)	LL50 (96 h): ca. 24 mg/L Water accommodated fraction (nominal) NOELR (96 h): ca. 3.2 mg/L Water accommodated fraction (nominal)	2 (reliable with restrictions) key study experimental result Test material (IUPAC name): Reaction products of bis(4-methylpentan-2-yl)dithiophosphoric acid with phosphorus oxide, propylene oxide and amines, C12-14-alkyl (branched)	Shacklady, L.G. (2001)
Pimephales promelas freshwater static OECD Guideline 203 (Fish, Acute Toxicity Test)	LC50 (96 h): ca. 8.5 mg/L test mat. (nominal)	2 (reliable with restrictions) supporting study experimental result Test material (IUPAC name): Reaction products of bis(4-methylpentan-2-yl)dithiophosphoric acid with phosphorus oxide, propylene oxide and amines, C12-14-alkyl (branched)	Timothy, J. Ward, R,, Boeri, L. (1998)
Pimephales promelas freshwater static OECD Guideline 203 (Fish, Acute Toxicity Test)	LC50 (96 h): ca. 19 mg/L test mat. (nominal)	2 (reliable with restrictions) supporting study experimental result Test material (IUPAC name): Reaction products of bis(4-methylpentan-2-yl)dithiophosphoric acid with phosphorus oxide, propylene oxide and amines, C12-14-alkyl (branched)	Morris, R.G., Holmes, C.M., Martin, K.H., and Swigert J.P (1993)

[3] ECHA (2013). Guidance on the Application of the CLP criteria – Guidance to Regulation (EC) No 1272/2008 on classification, labelling and packaging (CLP) of substances and mixtures. Version 4.0, November 2013

7.1.1.1.2 Long-term toxicity to fish

No data are available for this substance Justification for data waiving provided in Chemical Safety Report is following: in short-term tests the water flea demonstrated equivalent sensitivity to the test substance as compared to the fish, and given that the chronic water flea study covers the complete life cycle of the organism it was deemed sufficient to characterize the long term endpoint for aquatic organisms along with the chronic algae results.

However,further testing is not considered necessary to conclude on PBT (vPvB) assessment.

7.1.1.2 Aquatic invertebrates

7.1.1.2.1 Short-term toxicity to aquatic invertebrates

The results of the study are summarised in the following table:

Table 13: Overview of short-term effects on aquatic invertebrates

Method	Results	Remarks	Reference
Daphnia magna freshwater static OECD Guideline 202 (Daphnia sp. Acute Immobilisation Test)	EL50 (Loading rates) (48 h): ca. 91.4 mg/L test mat. (nominal) based on: mobility	2 (reliable with restrictions) key study experimental result Test material (IUPAC name): Reaction products of bis(4-methylpentan-2-yl)dithiophosphoric acid with phosphorus oxide, propylene oxide and amines, C12-14-alkyl (branched)	Blattenberger, R.F. (2002)

7.1.1.2.2 Long-term toxicity to aquatic invertebrates

The results of the study are summarised in the following table:

Table 14: Overview of long-term effects on aquatic invertebrates

Method	Results	Remarks	Reference
Daphnia magna	EL50 (21 d): 0.91 test mat. (nominal) based on: immobilisation	2 (reliable with restrictions)	Goodband, T. (2008)

Method	Results	Remarks	Reference
freshwater Other: renewed 3 times per week on Days 0, 2, 5, 7, 9, 12, 14, 16 and 19. OECD Guideline 211 (Daphnia magna Reproduction Test) EU Method C.20 (Daphnia magna Reproduction Test)	(For P1 Generation) EL50 (21 d): 0.66 mg/L test mat. (nominal) based on: reproduction (For F1 generation) NOEL (21 d): 0.12 mg/L test mat. (nominal) based on: immobilisation (for parental generation (P1)) NOEL (21 d): 0.12 mg/L test mat. (nominal) based on: reproduction (Based on numbers of live young produced per adult by Day 21)	key study experimental result Test material (IUPAC name): Reaction products of bis(4-methylpentan-2-yl)dithiophosphoric acid with phosphorus oxide, propylene oxide and amines, C12-14-alkyl (branched)	

7.1.1.3 Algae and aquatic plants

The results of the study are summarised in the following table:

Table 15: Overview of effects on algae and aquatic plants

Method	Results	Remarks	Reference
Selenastrum capricornutum (new name: Pseudokirchnerella subcapitata) (algae) freshwater static OECD Guideline 201 (Alga, Growth Inhibition Test)	EC_{50} (96 h): 6.4 mg/L test mat. (nominal) based on: cell number EC_{50} (96 h): 15 mg/L test mat. (nominal) based on: growth rate NOEC (96 h): 1.7 mg/L test mat. (nominal) based on: cell number NOEC (96 h): 3.3 mg/L test mat. (nominal) based on: growth rate	2 (reliable with restrictions) key study experimental result Test material (IUPAC name): Reaction products of bis(4-methylpentan-2-yl)dithiophosphoric acid with phosphorus oxide, propylene oxide and amines, C12-14-alkyl (branched)	Ward, T.J., Wyskiel, D.C. , Boeri, R.L (2000)

7.1.1.4 Sediment organisms

No data on toxicity to sediment organisms are available for this substance. Justification for data waiving provided in Chemical Safety Report is following: no data on the effect of the substance on sediment organisms are available. In accordance with REACH Annex X, section 9.5.1, testing is not warranted based on results of CSR. RCRs for freshwater and marine sediment are less than 1

even using conservative EUSES, thereby demonstrating negligible risk for sediment compartment. Testing results indicate low bioavailability and low toxicity potential. Based on the manner of use, exposure is not significant. Long term sediment toxicity testing is not necessary to derive PNEC sediment according to R.7.8.9.1; a read across from pelagic effect values is acceptable using equilibrium partitioning.

However,further testing is not considered necessary to conclude on PBT (vPvB) assessment.

7.1.1.5 Other aquatic organisms

No data on the effect of the substance on other aquatic organisms are available.

7.1.2 Calculation of Predicted No Effect Concentration (PNEC)

7.1.2.1 PNEC water

The derivation of the PNEC water is reported below. In the Chemical Safety Report an endpoint for algae based on cell number was considered in the PNEC derivation, whereas generally preference should be given to endpoints based on growth rate. The EC_{10} or NOEC from an algae test may be used as an additional long term result when other long-term data are available. Therefore, an assessment factor of 50 can be applied on the lowest NOEC instead of 100 as applied in the Chemical Safety Report.

Table 16: PNEC aquatic

	Value	Assessment factor	Remarks/Justification
PNEC aqua – freshwater (mg/L)	2.4×10^{-3}	50	Assessment factor based on the availability of two long term results
PNEC aqua - marine water (mg/L)	2.4×10^{-4}	500	Assessment factor based on the availability of two long term results
PNEC aqua – intermittent releases (mg/L)	0.085	100	Assessment factor based on the availability of acute studies for three different trophic levels (fish, Daphnia and algae; fish (*Pimephales promelas*) was the most sensitive species)

Long-term results representing two trophic levels are available for this substance, and the lowest NOEC was determined to be 0.12 mg/L. Using an assessment factor of 50 (as presented in REACH guidance document R.10 (May 2008)[4], the resulting $PNEC_{aquatic\text{- }freshwater}$ is 2.4×10^{-3} mg/L.

In the absence of data for marine species the $PNEC_{aquatic\text{-}marine\ water}$ has been calculated using freshwater data in lieu. Using an assessment factor of 500, proposed when long term results are available for two trophic levels (REACH guidance document R.10 (May 2008), the resulting $PNEC_{aquatic\text{- }marine\ water}$ is 2.4×10^{-4} mg/L.

[4] ECHA (2008). Guidance on information requirements and chemical safety assessment – Chapter R.10 Characterisation of dose-[concentration] response for environment.

The most sensitive freshwater species was the fish *Pimephales promelas*, with an EC_{50} of 8.5 mg/L. If exposure were to occur via intermittent releases, the $PNEC_{aquatic\ –\ intermittent\ releases}$ would be 0.085 mg/L (REACH guidance document R.10 (May 2008)).

7.1.2.2 PNEC sediment

The derivation of the PNEC sediment is reported below.

Table 17: PNEC sediment

	Value	Assessment factor	Remarks/Justification
PNEC sediment (mg/kg d.w.)	1.4 $x10^{-3}$ (when K_{OC} = 17.8) 3.13 (when K_{OC} = 1.2 x 10^5)	See equations below	EPM method

No data on sediment dwelling organisms are available or considered to be required. A reliable Koc value is available, so the PNEC sediment was estimated using the equilibrium partitioning method (EPM) using the following equations:

$PNEC_{sed} = (K_{susp\text{-}water}/RHO_{susp}) * PNEC_{water}*1000$

Where:

$K_{susp\text{-}water} = Fair_{susp} * K_{air\text{-}water} + Fwater_{susp} + Fsolids_{susp} * (Kp/1000) * RHO_{solid}$
K_{OC}= 17.8 to 1.2 x 10^5
Fraction of organic carbon = 0.1;
$K_P = K_{OC}$* fraction of organic carbon
RHO_{solid} = 2500 kg/m^3
Fai r_{susp} = 0
$Fwater_{susp}$ = 0.9
$Fsolid_{susp}$ = 0.1
RHO_{susp} = 1170 kg/m^3

PNEC values of 1.4 $x10^{-3}$ mg/kg (when K_{OC} = 17.8) to 3.13 mg/kg (when K_{OC} = 1.2 x 10^5) were derived.

7.2 Terrestrial compartment

7.2.1 Toxicity test results

Not relevant for this SEV.

7.2.1.1 Toxicity to soil macro organisms

No data on toxicity to soil macro organisms are available for this substance. Justification provided in Chemical Safety Report is included in Annex: Confidential information.

Further testing on toxicity to soil macro organisms is not considered necessary to conclude on PBT (vPvB) assessment.

7.2.1.2 Toxicity to terrestrial plants

No data on toxicity to terrestrial plants are available for this substance. Justification provided in Chemical Safety Report is included in Annex: Confidential information.

Further testing on toxicity to terrestrial plants is not considered necessary to conclude on PBT (vPvB) assessment.

7.2.1.3 Toxicity to soil micro-organisms

No data on toxicity to soil macro organisms are available for this substance. Justification provided in Chemical Safety Report is included in Annex: Confidential information.

Further testing on toxicity to soil micro- organisms is not considered necessary to conclude on PBT (vPvB) assessment.).

7.2.1.4 Toxicity to other terrestrial organisms

No data on the toxicity of the substance to other terrestrial organisms are available.

7.2.2 Calculation of Predicted No Effect Concentration (PNEC_soil)

The derivation of the PNEC soil is reported below.

Table 18: PNEC soil

	Value	Assessment factor	Remarks/Justification
PNEC soil (mg/kg.w.)	6.6×10^{-4} (when K_{OC} = 17.8) 2.54 (when K_{OC} = 1.2×10^{5})	See equations below	EPM method.

No data on soil dwelling organisms are available or considered to be required. A reliable Koc value is available for this substance, the $PNEC_{soil}$ was estimated using the equilibrium partitioning method (EPM) using the equations shown below:

$PNEC_{soil} = (K_{soil\text{-}water}/RHO_{soil}) * PNEC_{water}*1000$

Where:

$K_{soil\text{-}water} = Fair_{soil} * K_{air\text{-}water} + Fwater_{soil} + Fsolids_{soil} * (Kp/1000) * RHO_{solid}$
K_{OC}= 17.8 to 1.2 x 10^5
Fraction of organic carbon = 0.02;
$K_P = K_{OC}$* fraction of organic carbon
RHO_{solid}= 2500 kg/m3
$Fair_{soil}$ = 0
$Fwater_{soil}$ = 0.4 (worst case)
$Fsolid_{soil}$ = 0.6
RHO_{soil}= 1700 kg/m^3

7.3 Atmospheric compartment

No data on exposure of the atmospheric compartment are available for this substance. Justification provided in Chemical Safety Report is included in Annex: Confidential information.

7.4 Endocrine disrupting properties

Not evaluated.

7.5 Microbiological activity in sewage treatment systems

7.5.1 Toxicity to aquatic micro-organisms

An overview of study results provided in Chemical Safety Report is included in Annex: Confidential information.

7.5.2 PNEC for sewage treatment plant

The derivation of the PNEC soil in the Chemical Safety Report is reported below.

Table 19: PNEC sewage treatment plant

	Value	Assessment factor	Remarks/Justification
$PNEC_{STP}$ (mg/L)	24.33	100	Assessment factor based on the availability of an EC_{50} from a respiration inhibition test.

The 3-hour EC_{50} for activated sludge microorganisms was 2433 mg/L. Using an assessment factor of 100 (REACH guidance document R.10 (May 2008), the resulting PNEC_STP is 24.33 mg/L.

7.6 Non compartment specific effects relevant for the food chain (secondary poisoning)

The CA evaluation of the data in relation to the B or vB criterion is presented in Section 8.1.2.

Further testing on secondary poisoning is not considered necessary to conclude on PBT (vPvB) assessment.

7.6.1 Toxicity to birds

No data on toxicity to birds are available for this substance. Justification provided in Chemical Safety Report is included in Annex: Confidential information.

7.6.2 Toxicity to mammals

Not evaluated.

7.6.3 Calculation of PNEC oral (secondary poisoning)

Table 20: PNEC oral

	Value	Assessment factor	Remarks/Justification
PNEC oral (mg/kg food)	10	4 (AS) 2.5 (remain. diff.) 5 (intrasp.) 6 (durat. of exp.)	Assessment factor based on the availability of an NOAEL from a 28-day repeat dose test.

For 1-[bis(4-methylpentan-2-yloxy)phosphinothioylsulfanyl]propan-2-ol (constituent structure I) experimental aquatic BCF value was 436 for whole fish, indicating that this molecule has a low potential to bioaccumulate in aquatic and terrestrial organisms. Also the other representative structures are concluded to have a low bioaccumulation in fish (see Section 8.1.2 of this report). However, this material is not readily biodegradable, thus, it is necessary to consider whether the substance has a potential to cause toxic effects if accumulated in higher organisms. According to the mammalian toxicity data presented in section 5 of the Chemical Safety Report, this substance is not classified as Very Toxic (T+) or Toxic (T). Based on this information, non compartment-specific effects relevant for the food chain, and secondary poisoning is not considered likely to occur.

NOAEL of 150 mg/kg/d from the 28-day repeat dose toxicity test in rats was used to derive PNEC $_{oral}$. This value was converted to daily food intake by multiplying a factor of 20, total assessment factor of 300 was used, and $PNEC_{oral}$ of 10 mg/kg food was obtained.

7.7 Conclusion on the environmental classification and labelling

Based on the available environmental fate and ecotoxicological data for daphnids, fish and algae, this substance has acute aquatic toxicity between 1-10 mg/L in the most sensitive species, it is not readily biodegradable, and has a log P is <0.3 to >7.10; the BCF value is 436 in whole fish for one constituent. Therefore, this substance needs to be classified as toxic to the aquatic environment

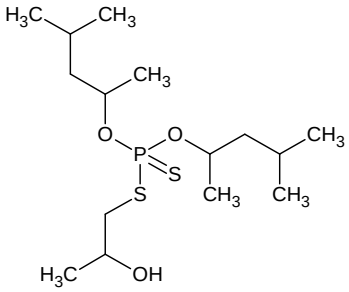
according to CLP Regulation (1272/2008/EC). This point is covered in Section 3.2 of this report as well.

8 PBT AND vPvB ASSESSMENT

8.1 Assessment of PBT/vPvB properties – Comparison with the criteria of Annex XIII

According to the guidance for the assessment of multi constituent substances in Section R.11.4.2.2 of the draft update of the ECHA PBT guidance document (ECHA, 2012b[5]) a PBT assessment has to be performed on the representative structures in an UVCB substance. The representative constituent structures were drawn with ADC/Chemsketch freeware[6] which enabled to search information on the exact structure via the internet. Key information on the representative structures for the substance under evaluation is summarized below. It should be noted that a number of constituents would occur in the environment only in an ionized form, whereas the information below might represent the non-dissociated structure.

Constituent structure I

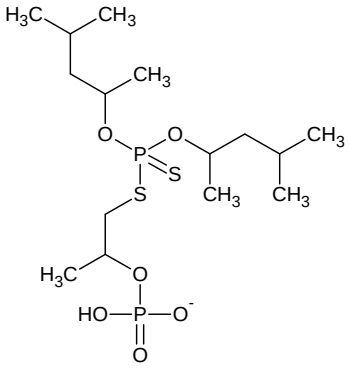


Molecular formula: $C_{15}H_{33}O_3PS_2$
Molecular weight: 356.52
SMILES notation: CC(C)CC(C)OP(=S)(OC(C)CC(C)C)SCC(C)O
IUPAC name: 1-[bis(4-methylpentan-2-yloxy)phosphinothioylsulfanyl]propan-2-ol
EC no: -
CAS no: -
PubChem code: CID13798195

[5] ECHA (2012b) Guidance on information requirements and chemical safety assessment – Chapter R.11: PBT and vPvB Assessment. Version 2.0, November 2012

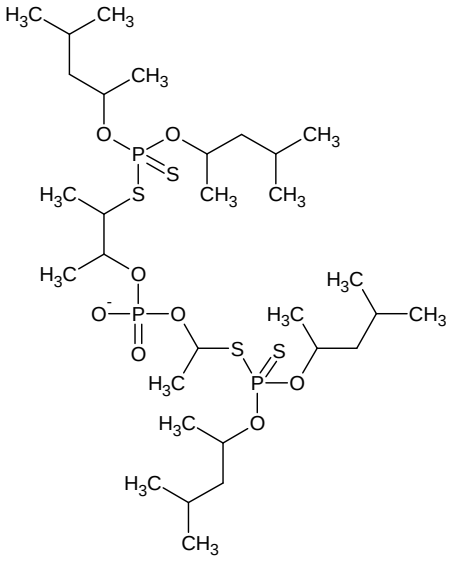
[6] ADC/Chemsketch freeware: ADC/Chemsketch for Professional and personal use. http://www.acdlabs.com/resources/freeware/chemsketch/

Constituent structure II



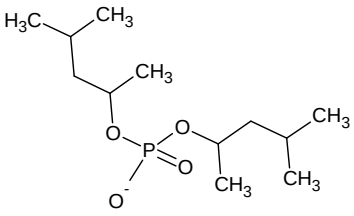
Molecular formula: $C_{15}H_{33}O_6P_2S_2$
Molecular weight: 435.50
SMILES notation: OP([O-])(=O)OC(C)CSP(=S)(OC(C)CC(C)C)OC(C)CC(C)C
IUPAC name: -
EC no: -
CAS no: -

Constituent structure III



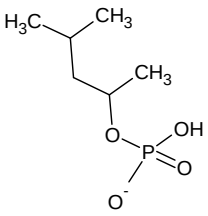
Molecular formula: $C_{30}H_{64}O_8P_3S_4$
Molecular weight: 774.0
SMILES notation: CC(C)CC(C)OP(=S)(OC(C)CC(C)C)SC(C)C(C)OP([O-])(=O)OC(C)SP(=S)(OC(C)CC(C)C)OC(C)CC(C)C
IUPAC name: -
EC no: -
CAS no: -

Constituent structure IV



Molecular formula: $C_{12}H_{26}O_4P$
Molecular weight: 265.31
SMILES notation: CC(C)CC(C)OP([O-])(=O)OC(C)CC(C)C
IUPAC name: Di (1,3-dimethylbutyl) phosphate
EC no: 282-415-9 (as phosphate ion), preregistered substance
CAS no: 84196-07-6

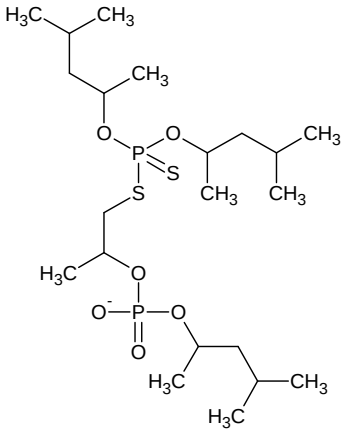
Constituent structure V



Molecular formula: $C_6H_{14}O_4P$
Molecular weight: 181.15
SMILES notation: [O-]P(=O)(O)OC(C)CC(C)C

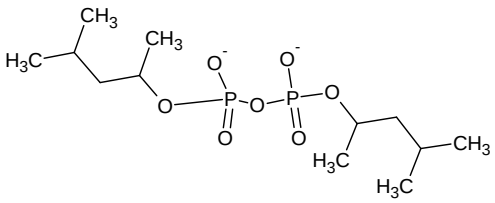
IUPAC name: 4-methylpentan-2-yl hydrogen phosphate
EC no: -
CAS no: -

Constituent structure VI



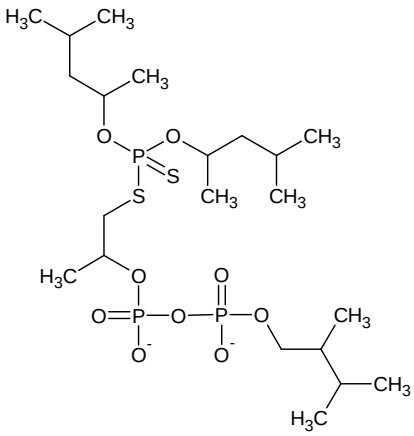
Molecular formula: $C_{21}H_{45}O_6P_2S_2$
Molecular weight: 519.66
SMILES notation: CC(C)CC(C)OP(=S)(OC(C)CC(C)C)SCC(C)OP([O-])(=O)OC(C)CC(C)C
IUPAC name: -
EC no: -
CAS no: -

Constituent structure VIIA



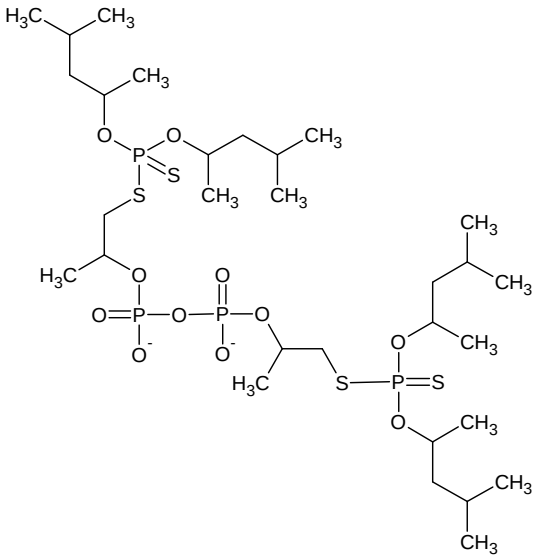
Molecular formula: $C_{12}H_{26}O_7P_2$
Molecular weight: 344.28
SMILES notation: CC(C)CC(C)OP([O-])(=O)OP([O-])(=O)OC(C)CC(C)C
IUPAC name: -
EC no: -
CAS no: -

Constituent structure VIIB



Molecular formula: $C_{21}H_{45}O_9P_3S_2$
Molecular weight: 598.63
SMILES notation: CC(C)CC(C)OP(=S)(OC(C)CC(C)C)SCC(C)OP([O-])(=O)OP([O-])(=O)OCC(C)C(C)C
IUPAC name: -
EC no: -
CAS no: -

Constituent structure VIIC



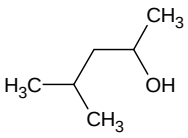
Molecular formula: $C_{30}H_{64}O_{11}P_4S_4$
Molecular weight: 852.98
SMILES not.: CC(C)CC(C)OP(=S)(OC(C)CC(C)C)SCC(C)OP([O-])(=O)OP([O-])(=O)OC(C)CSP(=S)(OC(C)CC(C)C)OC(C)CC(C)C
IUPAC name: -

EC no: -
CAS no: -

Constituent Amines, C12-C14-tert-alkyl

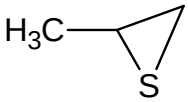
Molecular formula: mixture, not applicable
Molecular weight: mixture, not applicable
SMILES notation: mixture, not applicable
EC no: 273-279-1
CAS no: 68955-53-3

Constituent 4-methylpentan-2-ol



Molecular formula: $C_6H_{14}O$
Molecular weight: 102,174
SMILES notation: CC(C)CC(C)O
IUPAC name: 4-methylpentan-2-ol
EC no: 203-551-7
CAS no: 108-11-2

Constituent 1,2-epithiopropane



Molecular formula: C_3H_6S
Molecular weight: 74.14
SMILES notation: CC1CS1
IUPAC name: 1,2-methyl thiirane
EC no: 214-007-3
CAS no: 1072-43-1

Where data on the representative structure were lacking, read-across from data on similar structures was attempted following an analogue approach as defined in OECD guidance on grouping of chemicals (2007[7])

[7] OECD (2007a). Guidance on grouping of chemicals. OECD Series on Testing and Assessment Number 80. ENV/JM/MONO(2007)28

8.1.1 Persistence assessment

The substance under evaluation was not readily biodegradable. The Chemical Safety Report identified the substance as being potentially persistent, but only test results for the mixture are considered. According to the guidance for the assessment of multi constituent substances (R.11.4.2.2 Assessment of multi constituent substances) in the draft update of the ECHA PBT guidance document persistence assessment has to be performed on the representative structures in this UVCB substance that are present at ≥0.1% w/w. This assessment is reported below.

Constituent structure I
Constituent structure I falls in the category of dithiophosphate alkyl esters. A number of dithiophosphate alkyl esters were evaluated by EPA in the US High Production Volume Chemicals Program (EPA, 2009)[8]. This evaluation effectively followed the category approach described in OECD guidance on grouping of chemicals (OECD, 2007a).The evaluated category members in the dithiophosphate alkyl esters group were expected to show moderate to high persistence. Constituent structure I has the dithiophosphate functional group in common with many organophosphorous pesticidal active substances of which the environmental fate has been well studied. Comparable organophosphorous pesticidal active substances containing a dithiophosphate functional group and lacking halogen atoms or ring structures such as cadusofos, dimethoate, disulfoton, phorate and terbufos are not readily biodegradable, but at most showing moderate persistence in the environment. Given the higher molecular weight of constituent structure I compared to these substances a higher persistence might be expected and it cannot be excluded that it fulfils the criteria for either P or vP.

Constituent structure II
Constituent structure II falls in the category of dithiophosphate alkyl esters. A number of dithiophosphate alkyl esters were evaluated by EPA in the US High Production Volume Chemicals Program (EPA, 2009). The category members in the dithiophosphate alkyl esters group were expected to have moderate to high persistence. Constituent structure II has the dithiophosphate functional group in common with many organophosphorous pesticidal active substances of which the environmental fate has been well studied. Comparable organophosphorous pesticidal active substances containing a dithiophosphate functional group and lacking halogen atoms or ring structures such as cadusofos, dimethoate, disulfoton, phorate and terbufos are not readily biodegradable, but at most showing moderate persistence in the environment. Given the higher molecular weight of constituent structure II compared to these substances a higher persistence might be expected and it cannot be excluded that it fulfils endpoint criteria for either P or vP.

Constituent structure III
No experimental data or QSAR estimates of degradation are available for this substance. No data were found for similar structures combining thiophosphate and phosphate functional groups. Therefore, it cannot be excluded that it fulfils the criteria for either P or vP.

Constituent structure IV
Constituent structure IV falls in the category of phosphate alkyl esters. A number of phosphate alkyl esters were evaluated by EPA in the US High Production Volume Chemicals Program (EPA, 2009). The similar structure bis (2-ethylhexyl) phosphate exhibited in a biodegradability test appreciable biodegradation in 28 days or sooner indicating that the substance is moderately degradable and will not persist in the environment. It seems likely that di (1,3-dimethylbutyl) hydrogen phosphate will not fulfil endpoint criteria for either P or vP.

[8] EPA (2009). Screening level hazard characterization Dithiophosphate Alkyl Esters Category. U.S. EPA. High Production Volume (HPV) Challenge Program, December 2009.

Constituent structure V

Constituent structure V falls in the category of phosphate alkyl esters. A number of phosphate alkyl esters were evaluated by EPA in the US High Production Volume Chemicals Program (EPA, 2009). The similar structure ethylhexyl phosphate exhibited in a biodegradability test appreciable biodegradation in 28 days or sooner indicating that the substance is moderately degradable and will not persist in the environment. It seems likely that 4-methylpentan-2-yl dihydrogen phosphate will not fulfil endpoint criteria for either P or vP.

Constituent structure VI

No experimental data or QSAR estimates of degradation are available for constituent structure VI. No data were found for similar structures combining thiophosphate and phosphate functional groups. Therefore, it cannot be excluded that it fulfils endpoint criteria for either P or vP.

Constituent structure VIIA

No experimental data or QSAR estimates of degradation are available for constituent structure VIIA. Limited data are available for the organophosphorous pesticidal active substance tetraethyl pyrophosphate (TEPP) formerly used as an insecticide and containing a pyrophosphate functional group (Worthing, 1983[9]; TOXNET[10]). Based on summarised regulatory information TEPP is characterized as showing low persistence in the environment forming monoethyl, diethyl and triethyl orthophosphates and being rapidly metabolized in animals. Analogously constituent structure VIIA can be expected to rapidly degrade in the environment forming monophosphates. It seems likely that constituent structure VIIA will not fulfil endpoint criteria for either P or vP.

Constituent structure VIIB

No experimental data or QSAR estimates of degradation are available for this substance. Limited data are available for the organophosphorous pesticidal active substance tetraethyl pyrophosphate (TEPP) formerly used as an insecticide and containing a pyrophosphate functional group (Worthing, 1983; TOXNET). Based on summarised regulatory information TEPP is characterized as showing low persistence in the environment forming monoethyl, diethyl and triethyl orthophosphates and being rapidly metabolized in animals. Analogously constituent structure VIIB can be expected to rapidly degrade in the environment forming structures II and V. It seems likely that constituent structure VIIB will not fulfill endpoint criteria for either P or vP.

Constituent structure VIIC

No experimental data or QSAR estimates of degradation are available for this constituent containing a pyrophosphate functional group. Limited data are available for the organophosphorous pesticidal active substance tetraethyl pyrophosphate (TEPP) formerly used as an insecticide and containing a pyrophosphate functional group (Worthing, 1983; TOXNET). Based on summarized regulatory information TEPP is characterized as showing low persistence in the environment forming monoethyl, diethyl and triethyl orthophosphates and being rapidly metabolized in animals. Analogously constituent structure VIIC can be expected to rapidly degrade in the environment forming constituent structure II. It seems likely that constituent structure VIIC will not fulfil endpoint criteria for either P or vP.

Constituent amino salt of thiophosphate ester

This salt will rapidly dissociate in the environment, forming other constituents of the substance under evaluation.

[9] Worthing CR (1983). The Pesticide Manual – A world compendum. Seventh Edition. The British Crop Protection Council, 1983

[10] Toxnet:Hazardous Substances Data Bank (HSDB)

http://toxnet.nlm.nih.gov/cgi-in/sis/search/r?dbs+hsdb:@term+@na+TETRAETHYL%20PYROPHOSPHATE

Constituent Amines, C12-C14-tert-alkyl
The constituent is a mixture of predominantly branched C12-C14 alkyl amines also containing branched C10-C11 alkyl amines. PBT assessment is provided in the Chemical Safety Report.

Based on the ecotoxicological results, Amines, C12-C14-tert-alkylis not either P or vP.

Constituent 4-methylpentan-2-ol
4-methylpentan-2-ol is a registered substance. It was concluded to be readily biodegradable based on a reliable test in the Chemical Safety Report. Therefore, constituent 4-methylpentan-2-ol does not fulfil endpoint criteria for either P or vP.

Constituent 1,2-epithiopropane
No biodegradation data for 1,2-epithiopropane were found in publicly available MSDS information. Therefore, it cannot be excluded that it fulfils endpoint criteria for either P or vP.

8.1.2 Bioaccumulation assessment

According to the guidance for the assessment of multi constituent substances in the revised PBT guidance document a bioaccumulation assessment has to be performed on the representative structures in this UVCB substance that are present at ≥0.1% w/w. In the Chemical Safety Report bioaccumulation was assessed based on an experimental fish study for one constituent and BCF modelling for 11 other constituents (Gobas, 2005[11]). The results are evaluated below in conjunction with publicly available information on analogous substances.

Several methodologies were used to characterize or estimate the bioconcentration factor (BCF) of the constituent structures. These methods included:

(i) searches for empirical bioconcentration, bioaccumulation and K_{OW} data
(ii) estimation of the K_{OW} and KO_A for the constituent structures
(iii) estimation of the degradability of the constituent structures
(iv) estimation of the BCF using the BCFWIN model
(v) estimation of the metabolic transformation rate of the 11 compounds in fish
(vi) estimation of the BCF using the Gobas model

The SRC EFDB and BCF data bases and the Gobas and Arnot (2003)[12] BCF and BAF data base were searched for published data on the BCF, BAF and K_{OW} of constituent structures I to VIIC using the SMILES structures look up feature. The SRC BCF data base contains approximately 700 empirical BCF data. The Gobas and Arnot (2003) data base contains 5,092 BCF and 1,120 BAF entries for 773 chemicals. The data base pertaining to chemicals on the Canadian Domestic Substances List is published by Environment Canada on their website.
To estimate the potential for metabolic transformation of the constituent structures I to VIIC in fish, the Gobas and Arnot (2003) data base was explored for analogue substances. These are substances that have structural similarities to the constituent structures I to VIIC.
Constituent structures I to VIIC are all phosphate esters. Two types of phosphate esters, namely sulphur and non-sulphur containing substances, were distinguished. The constituent structures I to VIIC were divided in two classes and referred to as type 1 (constituent structure IV, V and VIIA)

[11] Gobas F.A.P.C., 2005. Assessment of the Bioconcentration Factors of 11 Compounds in Fish. Scholl of Resource & Environmental Management, Simon Frazer University, November 29, 2005.

[12] Gobas, F.A.P.C., J.A: Arnot. (2003) Categorizing of organic substances on the domestic substances list for bioaccumulation potential. Report to Environment Canada, Ottawa, p.110

and type 2 (constituent structures I, II, III. VI, VIIB and VIIC). The Gobas and Arnot (2003) data base includes 78 phosphate esters with comparable structures. Of these substances, 69 chemicals were identified that show strong structural similarities with the type 1 compounds and 9 substances that show similarities with the type 2 substances. Among the chemical substances that show structural similarities with the type 1 substances, there were 4 substances for which empirical bioconcentration data were available. Also, for the type 2 substances there were 4 substances in the data base with empirical bioaccumulation data. Empirical BCF data were plotted as a function of KOW in Figures 1 and 2. The Gobas (1993)[13] bioaccumulation model was then fitted to the empirical data to derive an apparent metabolic transformation rate constant for the type 1 and type 2 substances. This produced rate constants for type 1 and type 2 substances. These rate constants were then used in the Gobas 1993 model to estimate the contribution of metabolic transformation to the BCF for the type 1 and type 2 substances under investigation.

The BCF of the test chemicals was calculated using the Gobas 1993 model in a small fish (13 g) with a 5% lipid content at an ambient temperature of 10°C. The model calculations were conducted under two scenarios. The first scenario assumed that the test chemicals do not undergo metabolic transformation in fish, i.e. $k_M = 0\ d^{-1}$ in the model. This produces a conservative (i.e. highest possible) estimate of the BCF. In the second scenario, it was assumed that the test chemicals undergo metabolic transformation at rates consistent with the observed empirical BCFs of the analogue substances in the data base. This produced estimates of the BCF that recognize the inherent ability of the substances to be degraded in fish. This estimate of the BCF is expected to be more realistic than the one calculated under the scenario of no metabolic transformation. However, the uncertainty in the estimate of the actual BCF (i.e. the BCF with metabolism) is greater than that in the estimate of the maximum possible BCF. This is due to the fact that there are a large number of substances that support the ability of the model to estimate the maximum possible BCF while there are only a small number of data available from which the actual metabolic transformation rate can be inferred.

[13] Gobas, F.A.P.C. (1993). A model for predicting the bioaccumulation of hydrophobic organic chemicals in aquatic food webs: Application to Lake Ontario. Ecol. Modelling 69: 1-17.

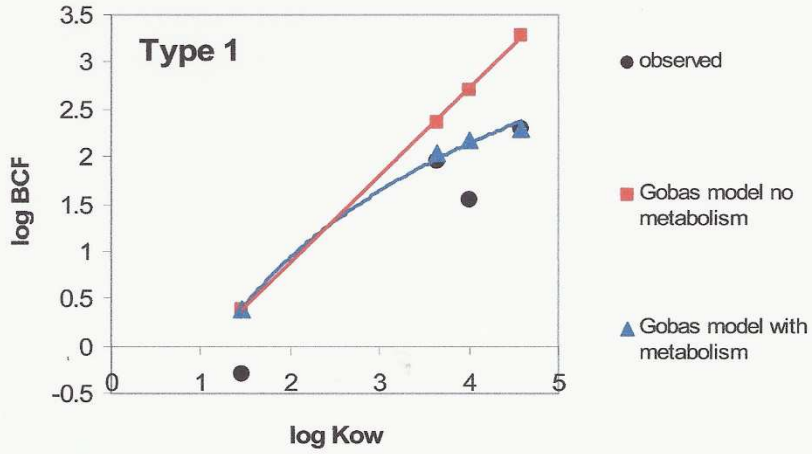


Figure 1 : Observed log BCF of type 1 analogue substances in relation to BCF model predictions using the Gobas model with or without metabolism.

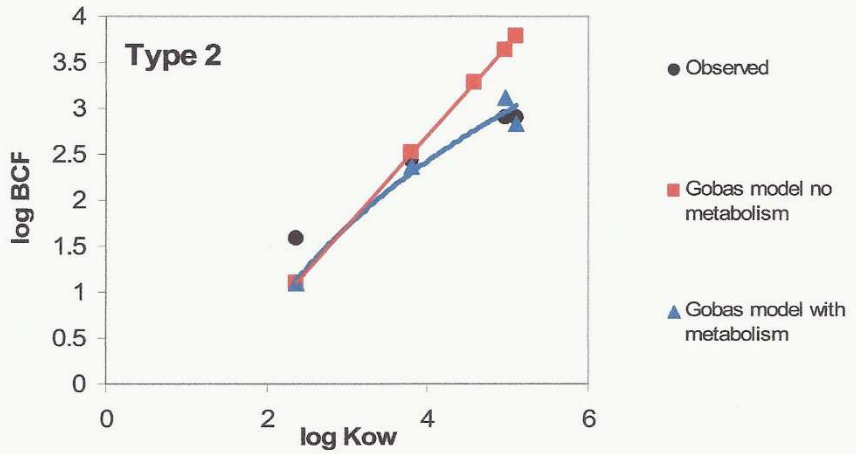


Figure 2 : Observed log BCF of type 2 analogue substances in relation to BCF model predictions using the Gobas model with or without metabolism.

According to OECD principles to facilitate the consideration of a (Q)SAR model for regulatory purposes, it should be associated with the following information (ENV/JM/MONO(2007)2[14]):

(i) a defined endpoint;
(ii) an unambiguous algorithm;
(iii) a defined domain of applicability;
(iv) appropriate measures of goodness-of-fit, robustness and predictivity;
(v) a mechanistic interpretation, if possible.

Based on these principles both the BCFWIN and the Gobas model can be considered adequate for regulatory purposes. The Gobas model with metabolism has a better defined and more targeted domain of applicability compared to the BCFWIN model. The fact that the model is validated with an experimental BCF for one of the constituent structures gives more confidence in the predictive value for other constituent structures.

It should be noted that the use of the BCF to estimate bioaccumulation potential has been criticized (f.i. Arnot & Gobas, 2006[15]). The BCF is not capable of meeting all environmental objectives because dietary exposure and other key environmental processes that may lead to higher chemical concentrations are not included.
A number of constituents would occur in the environment only in an ionized form, whereas estimates of hydrophobicity relate to the non-dissociated structure. Because of the significant reduction in hydrophobicity upon dissociation or protonation Kow values would require an appropriate correction to estimate the BCF of a compound with substantial degree of dissociation. The assessment below might thus overestimate the bioaccumulative properties for these constituents.

Constituent structure I
Constituent structure I was tested in a fish bioaccumulation study resulting in a steady state BCF in whole fish of 436 and a kinetic BCF in whole fish of 834 showing that it does not fulfil endpoint criteria for either B or vB. For constituent structure I estimated log BCF values in fish as reported in Gobas (2005) were 2.55 (BCFWIN), 4.53 (Gobas model, no metabolism) and 2.79 (Gobas model with metabolism), corresponding to BCF values of 355, 33,884 and 617, respectively. Compared to experimental BCF values above, this indicates a reasonable predictive value of both BCFWIN and the Gobas model with metabolism in the case of constituent structure I.

Constituent structure II
No experimental data are available for constituent structure II. Based on the structural similarity with constituent structure I a BCF in the same range might be expected. For constituent structure II estimated log BCF values in fish as reported in Gobas (2005) were 2.48 (BCFWIN), 4.50 (Gobas model, no metabolism) and 2.81 (Gobas model with metabolism), corresponding to BCF values of 302, 31,622 and 646, respectively. The reasonable predictive value of BCF estimates for constituent structure I is considered to support estimates for constituent structure II. For another dithiophosphate alkyl ester, cadusafos, the predicted BCF is 184 with the BCFWIN QSAR compared to an experimental value of 200 (whole fish) from a fish bioaccumulation study. This gives further support to the predictive value of BCFWIN in the case of dithiophosphate alkyl esters. The fact that the Gobas model with metabolism is validated with an experimental BCF for one of the constituent structures gives further confidence in the predictive value for constituent structure

[14] OECD (2007b). Guidance document on the validation of quantitative structure-activity relationship [(Q)SAR] models. OECD Environmental Health and Safety Publications – Series on testing and assessment No. 69, Paris, 2007

[15] Arnot J.A. & Gobas F.A.P.C. A review of bioconcentration factor (BCF) and bioaccumulation factor (BAF) assessment for orgnaic chemicals in aquatic organisms. Environm. Rev. 14: 257-297 (2006)

II. It is therefore reasonable to conclude that constituent structure II does not fulfil the criteria for either B or vB based on predicted BCF and supporting evidence.

Constituent structure III

No experimental data are available for constituent structure III. It has a molecular weight >700 g/mol which is an indicator that the aquatic BCF is lower than 5000 L/kg. Based on a calculated log Kow of 12.93 (KOWWIN) the aquatic BCF is probably lower than 2000 L/kg. The value of log Kow >10 is confirmed by the log Kow of 12.2 calculated with the help of ChemSketch and the related ADC/Labs model (ADC/Percepta Platform[16]) For constituent structure III estimated log BCF values in fish as reported in Gobas (2005) were 0.09 (BCFWIN), 0.08 (Gobas model, no metabolism) and -0.02 (Gobas model with metabolism). It is recognized that at very high log Kow (>6) the relationship between log Kow and BCF becomes very uncertain, but the results of both QSARs are in good agreement. The fact that the Gobas model with metabolism is validated with an experimental BCF for one of the constituent structures gives further confidence in the predictive value for constituent structure III. It is therefore reasonable to conclude that constituent structure III does not fulfil endpoint criteria for either B or vB based on predicted BCF values.

Constituent structure IV

No experimental data are available for constituent structure IV. For constituent structure IV estimated log BCF values in fish as reported in Gobas (2005) were 0.8 (BCFWIN), 2.95 (Gobas model, no metabolism) and 2.24 (Gobas model with metabolism). The calculated log Kow of 4.25 (BIOWIN) is below the screening criterion of 4.5. Therefore, di (1,3-dimethylbutyl) hydrogen phosphate does not fulfil endpoint criteria for either B or vB. Considering the outcome of the Gobas model this conclusion does not depend on the role of metabolism and has a high degree of certainty.

Constituent structure V

No experimental data are available for constituent structure V. For constituent structure V estimated log BCF values in fish as reported in Gobas (2005) were 0.64 (BCFWIN), 0.57 (Gobas model, no metabolism) and 0.56 (Gobas model with metabolism). The calculated log Kow of 1.74 (BIOWIN) is below the screening criterion of 4.5. Therefore, 4-methylpentan-2-yl dihydrogen phosphate does not fulfil the criteria for either B or vB. Considering the outcome of the Gobas model this conclusion does not depend on the role of metabolism and has a high degree of certainty.

Constituent structure VI

No experimental data are available for constituent structure VI. For constituent structure VI estimated log BCF values in fish as reported in Gobas (2005) were 0.5 (BCFWIN), 3.66 (Gobas model, no metabolism) and 1.08 (Gobas model with metabolism), corresponding to BCF values of 3.2, 4.71 and 12, respectively. The calculated value of log Kow of 8.59 (BIOWIN) is confirmed by the log Kow of 7.81 calculated with the help of ChemSketch and the related ADC/Labs model. It is recognized that at very high log Kow (>6) the relationship between log Kow and BCF becomes very uncertain. However, the result of the Gobas model including estimated metabolism is in good agreement with the BIOWIN estimate. The fact that the Gobas model with metabolism is validated with an experimental BCF for one of the constituent structures gives further confidence in the predictive value for constituent structure VI. It is therefore reasonable to conclude that constituent structure VI does not fulfil endpoint criteria for either B or vB.

Constituent structure VIIA

No experimental data are available for constituent structure VIIA. For constituent structure VIIA estimated log BCF values in fish as reported in Gobas (2005) were 1.05 (BCFWIN), 1.99 (Gobas

[16] ADC/Percepta platform: http://www.acdlabs.com/products/percepta/

model, no metabolism) and 1.83 (Gobas model with metabolism). The calculated log Kow of 3.28 (BIOWIN) is below the screening criterion of 4.5. Therefore, constituent structure VIIA does not fulfil endpoint criteria for either B or vB. Considering the outcome of the Gobas model this conclusion does not depend on the role of metabolism and has a high degree of certainty.

Constituent structure VIIB

For constituent structure VIIB estimated log BCF values in fish as reported in Gobas (2005) were 1.68 (BCFWIN), 4.24 (Gobas model, no metabolism) and 1.95 (Gobas model with metabolism), corresponding to BCF values of 48, 17.78 and 89, respectively. The calculated value of log Kow of 7.62 (BIOWIN) is confirmed by the log Kow of 6.54 calculated with the help of ChemSketch and the related ADC/Labs model. It is recognised that at very high log Kow (>6) the relationship between log Kow and BCF becomes very uncertain. However, the result of the Gobas model including estimated metabolism is in good agreement with the BIOWIN estimate. In Gobas (2005) it is acknowledged that the estimation of metabolic transformation in fish is rather uncertain, because rates of metabolic transformation in fish are poorly known and expected to show large variability among species and environmental conditions such as temperature. However, the rapid metabolism in animals of tetraethyl pyrophosphate (TEPP) which contains a pyrophosphate functional group like in constituent structure VIIB is considered supportive of considerable metabolism in fish. Constituent structure VIIB does not fulfil endpoint criteria for either B or vB. The fact that the Gobas model with metabolism is validated with an experimental BCF for one of the constituent structures gives further confidence in the predictive value for constituent structure VIIB.

Constituent structure VIIC

No experimental data are available for constituent structure VIIC. It has a molecular weight >700 g/mol which is an indicator that the aquatic BCF is lower than 5000 L/kg. Based on a calculated log Kow of 11.96 (KOWWIN) the aquatic BCF is probably lower than 2000 L/kg. The value of log Kow >10 is confirmed by the log Kow of 10.75 calculated with the help of ChemSketch and the related ADC/Labs model. For constituent structure VIIC estimated log BCF values in fish as reported in Gobas (2005) were 0.5 (BCFWIN), 0.56 (Gobas model, no metabolism) and -0.02 (Gobas model with metabolism). It is recognized that at very high log Kow (>6) the relationship between log Kow and BCF becomes very uncertain, but the results of both QSARs are in good agreement. It is therefore reasonable to conclude that constituent structure VIIC does not fulfil endpoint criteria for either B or vB based on predicted BCF and supporting evidence. Considering the outcome of the Gobas model this conclusion does not depend on the role of metabolism and has a high degree of certainty.

Constituent amino salt of thiophosphate ester

This salt will rapidly dissociate in the environment, forming other constituents of the substance under evaluation.

Constituent Amines, C12-C14-tert-alkyl

The constituent is a mixture of predominantly branched C12-C14 alkyl amines also containing branched C10-C11 alkyl amines. Amines, C12-C14-tert-alkylis a registered substance and a PBT assessment is provided in the Chemical Safety Report for this substance.

Based on the estimated BCFfish and BCFearthworm of 58.21 and 10.4, respectively, Amines, C12-C14-tert-alkyl is not either B or vB

Constituent 4-methylpentan-2-ol

4-methylpentan-2-ol is a registered substance and an estimated log Kow of 1.57 (ADC Lab service) is provided in the Chemical Safety Report. Therefore, constituent 4-methylpentan-2-ol does not fulfil endpoint criteria for either B or vB.

Constituent 1,2-epithiopropane

The estimated log Kow for 1,2-epithiopropane is 1.57 (ADC Lab service). Therefore, constituent 1,2-epithiopropane does not fulfil endpoint criteria for either B or vB.

8.1.3 Toxicity assessment

In the Chemical Safety Report the substance under evaluation was classified as not fulfilling endpoint criteria for T based on test results with the mixture. To assess whether the substance fulfils the T criterion in the PBT assessment toxicity endpoints based on WAF are for the substance under evaluation not considered appropriate. The results do not exclude that one or more constituents of the mixture fulfil endpoint criteria for T. According to the guidance for the assessment of multi constituent substances in the draft update of the PBT guidance document (ECHA, 2012b) a toxicity assessment has to be performed on the representative structures in this UVCB substance. This assessment is reported below.

Constituent structure I

No toxicity data or QSAR estimates of toxicity were found for this substance. Data are available for comparable organophosphorous pesticidal active substances containing a dithiophosphate functional group and lacking halogen atoms or ring structures. Cadusofos, dimethoate, disulfoton, phorate and terbufos are all toxic to very toxic to aquatic organisms. It is concluded that constituent structure I potentially fulfils endpoint criteria for T.

Constituent structure II

No toxicity data or QSAR estimates of toxicity were found for this substance. Data are available for comparable organophosphorous pesticidal active substances containing a dithiophosphate functional group and lacking halogen atoms or ring structures. Cadusofos, dimethoate, disulfoton, phorate and terbufos are all toxic to very toxic to aquatic organisms. It is concluded that constituent structure II potentially fulfils endpoint criteria for T.

Constituent structure III

No toxicity data or QSAR estimates of toxicity were found for this substance. Data are available for organophosphorous pesticidal active substances containing a dithiophosphate functional group and lacking halogen atoms or ring structures. Cadusofos, dimethoate, disulfoton, phorate and terbufos are all toxic to very toxic to aquatic organisms. It is concluded that constituent structure III potentially fulfils endpoint criteria for T.

Constituent structure IV

No toxicity data or QSAR estimates of toxicity were found for this substance. Constituent structure IV falls in the category of phosphate alkyl esters. A number of phosphate alkyl esters were evaluated by EPA in the US High Production Volume Chemicals Program (EPA; 2009). Studies of the ecotoxicity of the chemicals in this category indicate that none of the members are highly toxic to aquatic species. It is therefore reasonable to assume that di (1,3-dimethylbutyl) hydrogen phosphate will not fulfil endpoint criteria for T.

Constituent structure V

No toxicity data or QSAR estimates of toxicity were found for this substance. Constituent structure V is a mono-ester falling in the category of phosphate alkyl esters. A number of phosphate alkyl esters including the mono-ester ethylhexyl phosphate were evaluated by EPA in the US High Production Volume Chemicals Program (EPA, 2009). Studies of the ecotoxicity of the chemicals in this category indicate that none of the members are highly toxic to aquatic species. It is therefore reasonable to assume that 4-methylpentan-2-yl dihydrogen phosphate will not fulfil endpoint criteria for T.

Constituent structure VI

No toxicity data or QSAR estimates of toxicity were found for this substance. No data were found for similar structures combining thiophosphate and phosphate functional groups. Data are available for organophosphorous pesticidal active substances containing a dithiophosphate functional group and lacking halogen atoms or ring structures. Cadusofos, dimethoate, disulfoton, phorate and terbufos are all toxic to very toxic to aquatic organisms. It is concluded that constituent structure VI potentially fulfils endpoint criteria for T.

Constituent structure VIIA

No experimental data or QSAR estimates of toxicity were found for constituent structure VIIA. Limited data are available for the organophosphorous pesticidal active substance tetraethyl pyrophosphate (TEPP) formerly used as an insecticide and containing a pyrophosphate functional group (Worthing, 1983; TOXNET). Based on summarised regulatory information TEPP is characterized as highly toxic to aquatic organisms. It is concluded that constituent structure VI potentially fulfils endpoint criteria for T.

Constituent structure VIIB

No experimental data or QSAR estimates of toxicity were found for this substance. Limited data are available for the organophosphorous pesticidal active substance tetraethyl pyrophosphate (TEPP) formerly used as an insecticide and containing a pyrophosphate functional group (Worthing, 1983; TOXNET). Based on summarised regulatory information TEPP is characterized as highly toxic to aquatic organisms. It is concluded that constituent structure VI potentially fulfils endpoint criteria for T.

Constituent structure VIIC

No experimental data or QSAR estimates of toxicity were found for this substance. Limited data are available for the organophosphorous pesticidal active substance tetraethyl pyrophosphate (TEPP) formerly used as an insecticide and containing a pyrophosphate functional group (Worthing, 1983; TOXNET). Based on summarised regulatory information TEPP is characterized as highly toxic to aquatic organisms. Due to the large size of the molecule bioavailability might be limited, but based on available data it cannot be excluded that constituent structure VIIC fulfils endpoint criteria for T.

Constituent amino salt of thiophosphate ester

This salt will rapidly dissociate in the environment, forming other constituents of the substance under evaluation.

Constituent Amines, C12-C14-tert-alkyl

The constituent is a mixture of predominantly branched C12-C14 alkyl amines also containing branched C10-C11 alkyl amines. Amines, C12-C14-tert-alkyl is a registered substance and a PBT assessment is provided in the Chemical Safety Report.

Based on the toxicological results for this substance, Amines, C12-C14-tert-alkyl can be considered toxic.

Constituent 4-methylpentan-2-ol

4-methylpentan-2-ol is a registered substance and aquatic toxicity data are provided in the Chemical Safety Report. Based on the ecotoxicological results, 4-methylpentan-2-ol does not fulfil endpoint criteria for T.

Constituent 1,2-epithiopropane

No ecotoxicological data for 1,2-epithiopropane were found in publicly available MSDS information. Therefore, it cannot be excluded that it fulfils endpoint criteria for T.

8.1.4 Summary and overall conclusions on PBT and vPvB Properties

Constituent structure I is not considered a PBT or vBvP substance, since it does not fulfil the criteria for either B or vB.

Constituent structure II is not considered a PBT or vBvP substance, since it does not fulfil the criteria for either B or vB.

Constituent structure III is not considered a PBT or vBvP substance, since it does not fulfil endpoint criteria for either B or vB.

Constituent structure IV is not considered a PBT or vBvP substance, since it does not fulfil endpoint criteria for either B or vB and unlikely to fulfil endpoint criteria for P and T.

Constituent structure V is not considered a PBT or vBvP substance, since it does not fulfil endpoint criteria for either B or vB and unlikely to fulfil endpoint criteria for P and T.

Constituent structure VI is not considered a PBT or vBvP substance, since it does not fulfil the criteria for either B or vB.

Constituent structure VIIA is not considered a PBT or vBvP substance, since it does not fulfil endpoint criteria for either B or vB and it is not expected to fulfil endpoint criteria for P or vP.

Constituent structure VIIB is not considered a PBT or vBvP substance, since it does not fulfil endpoint criteria for either B or vB. In addition, it is not expected to fulfil endpoint criteria for P or vP.

Constituent structure VIIC is not considered a PBT or vBvP substance, since it does not fulfil endpoint criteria for either B or vB and not expected to fulfil endpoint criteria for P or vP.

Constituent Amines, C12-C14-tert-alkyl is not considered a PBT or vBvP substance, since it does not fulfil endpoint criteria for P, vP, B and vB.

Constituent 4-methylpentan-2-ol is not considered a PBT or vBvP substance, since it does not fulfil endpoint criteria for B, vB, P, vP and T.

Constituent 1,2-epithiopropane is not considered a PBT or vBvP substance, since the substance does not fulfil endpoint criteria for either B or vB.

In conclusion, the substance under evaluation is not considered a PBT or vBvP substance, since none of the constituents fulfils endpoint criteria for B or vB.

An overview of the conclusions:

	P	vP	B	vB	T	Fulfilling the PBT /vPvB criteria
Constituent structure I	Potentially	Potentially	No	No	Potentially	**No**
Constituent structure II	Potentially	Potentially	No	No	Potentially	**No**
Constituent structure III	Potentially	Potentially	No	No	Potentially	**No**
Constituent structure IV	No	No	No	No	No	**No**
Constituent structure V	No	No	No	No	No	**No**
Constituent structure VI	Potentially	Potentially	No	No	Potentially	**No**
Constituent structure VII A	No	No	No	No	Potentially	**No**
Constituent structure VII B	No	No	No	No	Potentially	**No**
Constituent structure VII C	No	No	No	No	Potentially	**No**
Constituent amines, C12-C14-tert-alkyl	No	No	No	No	Yes	**No**
Constituent 4-methylpentan-2-ol	No	No	No	No	No	**No**
Constituent 1,2-epithiopropane	Not excluded	Not excluded	No	No	Potentially	**No**
Constituent amino salt of thiophosphate ester	Not relevant for PBT/VPvB assessment (rapid dissociation in the environment)					**No**
Evaluated substance						**No**

9 EXPOSURE ASSESSMENT

Not evaluated.

10 RISK CHARACTERISATION

10.1 Human Health

Not evaluated.

10.2 Environment

10.2.1 Risk characterisation for PBT

The substance under evaluation is not considered a PBT or vPvB substance, since none of the constituents fulfils endpoint criteria for B or vB.

10.2.2 Aquatic compartment (incl. sediment)

Not evaluated.

10.2.3 Terrestrial compartment

Not evaluated.

10.2.4 Atmospheric compartment

Not evaluated.

10.2.5 Microbiological activity in sewage treatment systems

Not evaluated.

10.3 Overall risk characterisation

Not evaluated.

11 OTHER INFORMATION

None.

12 REFERENCES

ADC Chemsketch for Academic and Personal use:
http://www.acdlabs.com/resources/freeware/chemsketch/

ADC/Percepta platform: http://www.acdlabs.com/products/percepta/

Arnot J.A. & Gobas F.A.P.C. A review of bioconcentration factor (BCF) and bioaccumulation factor (BAF) assessment for orgnaic chemicals in aquatic organisms. Environm. Rev. 14: 257-297 (2006)

Conf. ref.1: (2013b). Chemistry description of EC No. 931-384.6. Interoffice Memorandum. September 26, 2013.

Conf. ref.2: (2013a). Updated identity summary for OS28526AB. Interoffice Memorandum February 2013, 26

Conf. ref.3: (2003). Separation and identification of Components of 0710.0 by HPLC and ESI-MS. Interoffice Memorandum 04JUN03

ECHA (2008). Guidance on information requirements and chemical safety assessment – Chapter R.10 Characterisation of dose-[concentration] response for environment.

ECHA (2012a). Guidance for indentification and naming of substances under REACH and CLP. Version: 1.2, March 2012

ECHA (2012b) Guidance on information requirements and chemical safety assessment – Chapter R.11: PBT and vPvB Assessment. Version 2.0, November 2012

ECHA (2013). Guidance on the Application of the CLP criteria – Guidance to Regulation (EC) No 1272/2008 on classification, labelling and packaging (CLP) of substances and mixtures. Version 4.0, November 2013

EPA (2009). Screening level hazard characterization Dithiophosphate Alkyl Esters Category. U.S. EPA. High Production Volume (HPV) Challenge Program, December 2009.

Gobas, F.A.P.C. (1993). A model for predicting the bioaccumulation of hydrophobic organic chemicals in aquatic food webs: Application to Lake Ontario. Ecol. Modelling 69: 1-17.

Gobas F.A.P.C., 2005. Assessment of the Bioconcentration Factors of 11 Compounds in Fish. Scholl of Resource & Environmental Management, Simon Frazer University, November 29, 2005.

Gobas, F.A.P.C., J.A: Arnot. (2003) Categorizing of organic substances on the domestic substances list for bioaccumulation potential. Report to Environment Canada, Ottawa, p.110

OECD (2000). Guidance document on aquatic toxicity testing of difficult substances and mixtures. OECD Series on Testing and Assessment Number 23, ENV/JM/MONO(2000)6.

OECD (2007). Guidance on grouping of chemicals. OECD Series on Testing and Assessment Number 80. ENV/JM/MONO(2007)28

PubChem: http://pubchem.ncbi.nlm.nih.gov/

Toxnet:Hazardous Substances Data Bank (HSDB): http://toxnet.nlm.nih.gov

Worthing, ed. (1983). The Pesticide Manual - A World Compendium. 7th ed. Lavenham, Suffolk, Great Britain: The Lavenham Press Limited, 1983.)

13 ABBREVIATIONS

BCF	Bioconcentration factor
CAS	Chemical Abstracts Service
CSR	Chemical Safety Report
CLP	Classification, Labelling and Packaging (of hazardous chemicals)
DNEL	Derived No Effect Level
ECHA	European Chemicals Agency
EPA	Environmental Protection Agency
ERC	Environmental Release Category
ESI-MS	Electrospray Ionization mass spectrometry
GHS	Globally Harmonized System (of Classification and Labelling of Chemicals)
HPLC	High-performance liquid chromatography
IUCLID	International Uniform Chemical Information Database
IUPAC	International Union of Pure and Applied Chemistry
CA	Competent Authority
NOAEL	No Observable Adverse Effect Level
OECD	Organization for Economic Cooperation and Development
QSAR	Quantitative Structure-Activity Relationship

PBT	Persistent Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
RCR	Risk Characterization Ratio
RMO	Risk Management Options
SEV	Substance Evaluation
TEPP	Tetraethyl pyrophosphate
UVCB	Substances of Unknown or Variable composition, Complex reaction products or Biological materials.
vPvB	Very Persistent and Very Bioaccumulative
WAF	Water-accommodated fraction

ANNEX: CONFIDENTIAL INFORMATION