

TETRAKIS(HYDROXYMETHYL)PHOSPHONIUM SULFATE

This dossier on tetrakis(hydroxymethyl)phosphonium sulfate (THPS) presents the most critical studies pertinent to the risk assessment of its use in drilling muds, hydraulic fracturing fluids and water treatment. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the IPCS Environmental Health Criteria document on flame retardants, which included THPS (IPCS, 2000). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – THPS is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

THPS is inherently biodegradable (not readily biodegradable). It is not expected to bioaccumulate, and it has a low to moderate potential to adsorb to soil and sediment. THPS has a high acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): bis[tetrakis(hydroxymethyl)phosphonium] sulfate

CAS RN: 55566-30-8

Molecular formula: C₈H₂₄O₈P₂O₄S

Molecular weight: 406.28 g/mol

Synonyms: Tetrakis(hydroxymethyl)phosphonium sulfate; bis[tetrakis(hydroxymethyl)phosphonium] sulfate; Octakis (hydroxymethyl) phosphonium sulfate; Tolcide PS75; THPS

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of THPS (75% solution)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless liquid	1	ECHA
Boiling Point	108.5°C @ 101.3 kPa	1	ECHA
Density	1390 kg/m ³ @ 20°C	1	ECHA
Vapour Pressure	Negligible	1	ECHA
Partition Coefficient (log K _{ow})	-9.8 (calculated) (temperature not provided)	2	ECHA
Water Solubility	37,700 g/L @ 21 °C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for THPS.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

THPS is inherently biodegradable (not readily biodegradable). It is not expected to bioaccumulate, and it has a low to moderate potential to adsorb to soil and sediment.

B. Partitioning

THPS is highly soluble in water. Volatilisation from [water](#) surfaces or moist soil surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant of 1.7×10^{-18} Pa m³/mol. It is also not expected to volatilise from dry soil surfaces based upon its vapor pressure (Pub Chem).

Hydrolysis is expected to be an important environmental fate process since this compound contains functional groups that hydrolyze under environmental conditions (pH 5 to 9) (PubChem). The hydrolysis of THPS is pH-dependent: half-lives at 25°C were 131, 72, and 7 days at pH 5, 7, and 9, respectively (IPCS, 2000).

C. Biodegradation

THPS is inherently biodegradable. In an OECD 302B study, >20% degradation occurred within a 28-day period (IPCS, 2000). Aquatic aerobic degradation of THPS was assessed in a soil/water system using USEPA guidelines. The soil was dosed with THPS at 1 µg/g. Radiolabelled THPS was metabolised with 60% of applied radioactivity appearing as CO₂ within 7 days. Major metabolites were trihydroxymethyl phosphine oxide (THPO) and bishydroxymethyl phosphonic acid (BMPPA), which were both found in the water; neither degradate reached a concentration of 10% of the applied dose (IPCS, 2000). A comparable study at the same initial concentration of THPS but under

anaerobic conditions also showed 60% degradation within 30 days, and the same breakdown products were identified (IPCS, 2000).

If a chemical is found to be inherently biodegradable or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

The estimated K_{oc} values estimated from tested soil and sediment samples using radiolabelled THPS ranged from 72 to 266, with a mean value of 153. The samples included sand, silt loam, sandy loam, pond sediment, and marine sediment (IPCS, 2000). Based on these estimated values, THPS is expected to be mobile to moderately mobile in soil. If released to water, based on the K_{oc} value and its high water solubility, it is also not expected to adsorb to suspended solids and sediment.

E. Bioaccumulation

There are no bioaccumulation studies on THPS. THPS is not expected to bioaccumulate based on a $\log K_{ow}$ of -9.8 (IPCS, 2000).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

THPS has a high acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on THPS.

Table 3 Acute Aquatic Toxicity Studies on THPS

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
<i>Oncorhynchus mykiss</i>	96-hr LC ₅₀	71	1	ECHA
<i>Lepomis macrochirus</i>	96-hr LC ₅₀	74	1	ECHA
<i>Cyprinodon variegatus</i>	96-hr LC ₅₀	72	1	ECHA
<i>Daphnia magna</i>	48-hr EC ₅₀	11.3	1	ECHA
		14.3	2	
<i>Lemna minor</i>	7 day EC ₅₀	1.5	1	ECHA

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

The LD₅₀ to mallard duck (*Anas platyrhynchos*) is 311 mg/kg (IPCS, 2000). The dietary LC₅₀ values to mallard ducks and bobwhite quail are 1,313 and 2,414 mg/kg diet, respectively (IPCS, 2000).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

THPS is inherently biodegradable. In an aquatic aerobic degradation system, radiolabelled THPS was metabolised with 60% of applied radioactivity appearing as CO₂ within 7 days. Thus, THPS does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of -9.8, THPS does not meet the screening criteria for bioaccumulation.

There are no chronic aquatic toxicity studies on THPS. While the single lowest acute EC₅₀ value for THPS is >1 mg/L and the remaining four toxicity test data for fish and invertebrates are orders of magnitude greater than the 1 mg/L screening criterion for toxicity. Thus, THPS is not considered to meet the screening criteria for toxicity.

The overall conclusion is that THPS is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for THPS.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment ¹	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required ³
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity ²	Chronic Toxicity ²	
Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8	Not a PBT	No	No	No	No	No	No	1	No data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 1 - Hazard Assessment only based on the preponderance of test data greatly exceeding the toxicity screening criterion

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

- Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.
- Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.
- ECHA. ECHA REACH database: <http://echa.europa.eu/information-on-chemicals/registered-substances>
- European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.
- Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.
- IPCS (2000). Flame Retardants: Tris(2-butoxyethyl)phosphate, Tris (2-ethylhexyl) phosphate and tetrakis (hydroxymethyl)phosphonium Salts, Environmental Health Criteria 218, International Programme on Chemical Safety, United Nations Environment Programme, International Labour Organisation, World Health Organization.
- PubChem. National Institutes of Health. National Library of Medicine National Center for Biotechnology Information. <https://pubchem.ncbi.nlm.nih.gov/>

B. Abbreviations and Acronyms

°C	degrees Celsius
µg/g	microgram per gram
AICS	Australian Inventory of Chemical Substances
BMPA	bishydroxymethyl phosphonic acid
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre

IUPAC	International Union of Pure and Applied Chemistry
kg/m ³	kilograms per cubic metre
KI	Klimisch scoring system
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
mm	millimetre
NOEC	no observed effects concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
THPO	trihydroxymethyl phosphine oxide
THPS	tetrakis(hydroxymethyl)phosphonium sulfate
USEPA	United States Environmental Protection Agency