

AMINO TRIMETHYLENE PHOSPHONIC ACID (ATMPA)

This dossier on amino trimethylene phosphonic acid (ATMPA) presents the most critical studies pertinent to the risk assessment of ATMPA in its use in coal seam gas extraction activities. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

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

1 BACKGROUND

ATMPA is a mineral-binding and complexing agent, with unusual chemical properties. The properties of ATMPA and its salts are profoundly affected by their ionisation behaviour. Each of the three phosphonic acid groups in ATMPA can ionise by loss of one or two hydrogen ions; in addition, the amine nitrogen can be protonated. Therefore, it is a strong complexing agent, and is highly hydrophilic.

ATMPA is not readily or inherently biodegradable. However, in the natural environment the fate and behaviour of ATMPA and its ions are dominated by abiotic dissociation/complexing, irreversible adsorption to surfaces, more than by degradation processes (ECHA). If released to water, ATMPA and its salts will partition primarily to water and suspended sediments. However, it has a low potential for bioaccumulation.

ATMPA is of low toxicity to aquatic organisms on an acute and chronic basis.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): nitrilotrimethylenetris(phosphonic acid)

CAS RN: 6419-19-8

Molecular formula: C₃H₁₂NO₉P₃

Molecular weight: 299.05 g/mol

Synonyms: Amino trimethylene phosphonic acid (ATMPA); aminotrimethylene phosphonic acid; phosphonic acid, [nitrilotris(methylene)]tris-; 1,1,1-nitrilotris(methylphosphonic acid)

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 ATMPA

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Yellow viscous liquid	2	ECHA
Melting Point	177.85°C @ 101.3 kPa	1	ECHA
Boiling Point	Decomposes without boiling	-	ECHA
Density	1330 kg/m ³ @ 20°C	2	ECHA
Vapour Pressure	2.7x10 ⁻⁹ Pa @ 25°C	2	ECHA
Partition Coefficient (log K _{ow})	-3.5	2	ECHA
Water Solubility	500 g/L @ 20°C	2	ECHA
Dissociation Constant (pKa)	<2 – 12.3 @ 20°C	2	ECHA

The properties of ATMPA and its salts are profoundly affected by their ionisation behaviour. Each of the three phosphonic acid groups in ATMPA can ionise by loss of one or two hydrogen ions; in addition, the amine nitrogen can be protonated. Therefore, it is a strong complexing agent, and is highly hydrophilic. Because ionisation is a rapid and reversible process, salts such as sodium and potassium will dissolve and dissociate readily in water to give a speciation state dictated by the pH of the medium (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 ATMPA.

NICNAS has assessed ATMPA in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health¹.

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

¹ <https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=6419-19-8>

Convention, Protocol or other international control	Listed Yes or No?
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

ATMPA is a mineral-binding and complexing agent, with unusual chemical properties. ATMPA and its salts adsorb strongly to soils and sediments despite the very low log K_{ow} of -3.5. The nature of the adsorption is believed to be primarily due to interaction with inorganic substrate or generalised surface interactions. For example, the presence of calcium in solution tends to significantly increase the adsorption of ATMPA. In natural waters this will play a part in the fate of ATMPA, particularly in slightly alkaline waters, as this represents a route of abiotic removal from the environment (ECHA).

While some biodegradation has been observed, the results of aerobic and anaerobic biodegradation studies for ATMP acid and its salts do not show significant biodegradation in the short term, and they are not readily or inherently biodegradable. In reliable ready biodegradability studies, 0 - 23% degradation was observed in 28 days (ECHA) [KI Score = 1 or 2, depending on the study].

Based on these factors and that ATMPA is hydrophilic, if released to water, ATMPA and its salts will partition primarily to water and suspended sediments. However, based on the measured BCF 22 L/kg in *Cyprinus carpio*, ATMPA is not expected to bioaccumulate (ECHA) [KI. Score = 2].

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

ATMPA is of low toxicity to aquatic organisms on an acute and chronic basis.

B. Aquatic Toxicity

Acute Studies

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

Table 3 Acute Aquatic Toxicity Studies on ATMPA

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
<i>Salmo gairdneri</i> (now known as <i>Oncorhynchus mykiss</i>) (Rainbow Trout)	96-hour LC ₅₀	160	1	ECHA
<i>Daphnia magna</i>	48-hour EC ₅₀	297	1	ECHA
<i>Pseudokircheriella subcapitata</i> (freshwater algae)	96-hour EC ₅₀	12.39 (biomass)	3*	ECHA
<i>Skeletonema costatum</i> (marine diatom)	72-hour EC ₅₀	80 (growth rate)	2	ECHA

*Assigned a Kl. Score of 3 due to deviations in pH in the higher concentrations used in the study. Furthermore, this study used a non-standard exposure duration and is based on biomass.

Chronic Studies

Table 4 Chronic Aquatic Studies on ATMPA

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
<i>Oncorhynchus mykiss</i> (Rainbow Trout)	60-day NOEC	23	1	ECHA
<i>Daphnia magna</i>	28-day NOEC	≥25	2	ECHA

C. Terrestrial Toxicity

No reliable studies are available for ATMPA on terrestrial (soil-dwelling) organisms or plants.

A short-term (14-day) LC₅₀ value of >565 mg active acid/kg bw has been determined for the effects of ATMPA on mortality of mallard duck (*Anas platyrhynchos*) (ECHA) [Kl. Score = 2]..

A short-term (14-day) LD₅₀ value of >2510 mg/kg bw/day, equivalent to >565 mg active acid/kg bw/day, has been determined for the effects of ATMP-H on mortality of bobwhite quail (*Colinus virginianus*) (ECHA). [Kl. Score = 2].

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).

ATMPA is not readily or inherently biodegradable. However, in the natural environment the fate and behaviour of ATMPA and its ions are dominated by abiotic dissociation/complexing, irreversible adsorption to surfaces, more than by degradation processes (ECHA). Thus, ATMPA does not meet the screening criteria for persistence.

The experimental BCF for ATMPA is < 22 L/kg. Thus, ATMPA does not meet the criteria for bioaccumulation.

The lowest NOEC from chronic aquatic toxicity studies is >0.1 mg/L. The acute EC₅₀ values for ATMPA are >1 mg/L in fish, invertebrates and algae. Thus, ATMPA does not meet the screening criteria for toxicity.

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

B. Other Characteristics of Concern

No other characteristics of concern were identified for ATMPA.

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	
Amino Trimethylene Phosphonic Acid	6419-19-8	Not a PBT	No	No	No	No	No	No	1	1	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.

Notes:

NA = not applicable

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.

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.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
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
kPa	kilopascal
LC	lethal concentration
L/Kg	litres per kilogram
mg/L	milligrams per litre
NOEC	no observed effects concentration
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases