

N,N-DIMETHYLMETHANAMINE

This dossier on N,N-dimethylmethanamine (trimethylamine) presents the most critical studies pertinent to the risk assessment of N,N-dimethylmethanamine in its use in hydraulic fracturing fluids. 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 – N,N-dimethylmethanamine (trimethylamine) is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

N,N-dimethylmethanamine is readily biodegradable. It is unlikely to bioaccumulate; and it will not adsorb significantly to suspended solids and sediments in water and is highly mobile in soil. N,N-dimethylmethanamine has low acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): trimethylamine

CAS RN: 75-50-3

Molecular formula: C₃H₉N or (CH₃)₃N

Molecular weight: 59.11 g/mol

Synonyms: N,N-dimethylmethanamine; trimethylamine; methanamine, N,N-dimethyl- (9CI); N-trimethylamine

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 N,N-dimethylmethanamine

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Liquified gas @ 20°C, with a pungent, fish ammonia-like odour	1	ECHA
Melting Point	-117.3°C to -117°C	2	ECHA
Boiling Point	2.9 to 3.5°C @ 101.3 kPa	2	ECHA
Density	630 to 670 kg/m ³ @ 20°C	2	ECHA
Vapour Pressure	190900 Pa @ 20°C 214600 Pa @ 25°C	2	ECHA

Property	Value	Klimisch score	Reference
Partition Coefficient (log K _{ow})	0.245 (pH 10 @ 25°C) <-3.5 (pH 7 with HCl @ 25°C)	2	ECHA
Water Solubility	409 g/L @ 19°C	2	ECHA
Dissociation Constant (pKa)	9.8 @ 20°C	2	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 N,N-dimethylmethanamine.

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

N,N-dimethylmethanamine is readily biodegradable. It unlikely to bioaccumulate; and it will not adsorb significantly to suspended solids and sediments in water and is highly mobile in soil.

B. Partitioning

N,N-dimethylmethanamine is highly soluble in water. Based on its Henry's Law Constant volatilisation from water or moist soil surfaces is not expected to be an important fate process. It is expected to volatilize from dry soil surfaces based upon its vapour pressure.

C. Biodegradation

N,N-dimethylmethanamine is readily biodegradable. In a OECD 301 C test, degradation was 92% in 14 days (ECHA). [Kl. score = 2]

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

D. Environmental Distribution

No experimental data are available for N,N-dimethylmethanamine. Using KOCWIN in EPISUITE™ (USEPA, 2017), the estimated K_{oc} value from $\log K_{ow}$ is 8.876 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 7.32 L/kg.

If released to soil, based on this estimated K_{oc} value, N,N-dimethylmethanamine is expected to have very high mobility. The pK_a of trimethylamine is 9.8 (PubChem), indicating that this compound will exist almost entirely in the cation form in the environment and cations generally adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts. If released into water, N,N-dimethylmethanamine is also not expected to adsorb to suspended solids and sediment based upon the estimated K_{oc} and its high solubility.

E. Bioaccumulation

No bioconcentration studies have been conducted on N,N-dimethylmethanamine. N,N-dimethylmethanamine is not expected to bioaccumulate based on the experimental $\log K_{ow}$ of <-3.5 at pH 7 (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

N,N-dimethylmethanamine has low acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on N,N-dimethylmethanamine.

Table 3 Acute Aquatic Toxicity Studies on N,N-dimethylmethanamine

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
<i>Leuciscus idus</i>	48-hr LC_{50}	25 (un-neutralised) 610 (neutralised)	2	ECHA
<i>Daphnia magna</i>	48-hr EC_{50}	139.95	2	ECHA
<i>Desmodesmus subspicatus</i>	72-hr EC_{50} EC_{10}	150 (growth rate) 90.6 (biomass) 86 (growth rate) 42.6 (biomass)	2	ECHA

Chronic Studies

Table 4 lists the results of chronic aquatic toxicity studies on N,N-dimethylmethanamine.

Table 4 **Chronic Aquatic Toxicity Studies on N,N-dimethylmethanamine**

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
<i>Daphnia magna</i>	EC ₁₀	3.9	2	ECHA

No chronic studies were available for fish or algae.

C. Terrestrial Toxicity

No studies are available.

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).

N,N-dimethylmethanamine is readily biodegradable; thus it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of <-3.5 at pH 7, N,N-dimethylmethanamine does not meet the screening criteria for bioaccumulation.

The EC₁₀ values from the chronic aquatic toxicity studies on N,N-dimethylmethanamine are >0.1 mg/L for invertebrates. There are no chronic toxicity studies on N,N-dimethylmethanamine for fish or algae. The acute E(L)C₅₀ values of N,N-dimethylmethanamine are >1 mg/L for fish, invertebrates and algae. Thus N,N-dimethylmethanamine does not meet the screening criteria for toxicity.

The overall conclusion is that N,N-dimethylmethanamine is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for N,N-dimethylmethanamine.

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	
N,N-dimethylmethanamine	75-50-3	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.

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.
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- USEPA. (2017). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: <https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface>.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
atm m ³ /mol	Atmosphere cubic meter per mol
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
hPa	hectopascal

IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
kg/m ³	kilogram per cubic metre
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases