DIETHANOLAMINE

This dossier on diethanolamine (DEA) presents the most critical studies pertinent to the risk assessment of diethanolamine in its use in hydraulic fracturing fluids. This dossier 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 –Diethanolamine is classified as a **tier 1** chemical and requires a hazard assessment only. A review of aquatic toxicity data indicates that overall (18 of 26 acute and chronic tests reviewed in ECHA) would classify the substance as tier 1. Moreover, the substance has been determined to biodegrade in the environment very quickly suggesting that chronic toxicity would be less relevant than acute toxicity (where 15 of 17 tests support the tier 1 classification).

1 BACKGROUND

Diethanolamine is readily biodegradable. It is not expected to bioaccumulate; and it has low potential to adsorb to soil. Diethanolamine exhibits moderate acute toxicity to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2,2'-iminodiethanol

CAS RN: 111-42-2

Molecular formula: $C_4H_{11}NO_2$

Molecular weight: 105.14 gm/mol

Synonyms: Diethanolamine; 2,2'-iminodiethanol; 2,2'-dihydroxydiethylamine; 2-[(2-hydroxyethyl)amino]ethanol; bis(2-hydroxyethyl)amine; DEA; di(2-hydroxyethyl)amine; ethanol, 2,2'-iminobis-(9Cl); ethanol, 2,2'iminodi-(8Cl)

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 Diethanolamine

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Solid Crystals (prisms) or syrupy liquid	2	ECHA
Melting Point	27°C @ 101.3 kPa	1	ECHA
Boiling Point	268.9°C (decomposition occurs >200°C) @ 101.3 kPa	1	ECHA

Property	Value	Klimisch score	Reference
Density	1100 kg/m^3 @ 20°C	2	ECHA
Vapour Pressure	0 Pa @ 20°C	2	ECHA
Partition Coefficient (log K_{ow})	-2.46 @ 25°C	2	ECHA
Water Solubility	1000 g/L @ 20 °C (miscible)	2	ECHA
Dissociation Constant (pKa)	8.99 @ 20°C	2	ECHA
Viscosity	390.9 mPa.s @ 30°C; 102.7 mPa.s @ 50°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 diethanolamine.

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

Diethanolamine is readily biodegradable. It is not expected to bioaccumulate, and it has low potential to adsorb to soil.

B. Partitioning

Diethanolamine is highly soluble in water. Based on its Henry's Law Constant is not expected to evaporate into the atmosphere from the water surface. However, the substance will be rapidly degraded by photochemical processes (half-life = 4.2 h).

C. Biodegradation

Diethanolamine is readily biodegradable. In an OECD 301F test, there was 50% degradation after 7 days, 80% after 14 days, and 93% after 28 days (OECD, 2007; ECHA) [Kl. score = 1]. In a "Ready"

Biodegradability – Dissolved Organic Carbon (DOC) Die-Away test, there was 86% degradation after 7 days and 96% degradation after 10 days (ECHA) [Kl. score = 2]. In modified OECD 301E screening tests using river or pond water, there was 93% and 97% degradation (measured as DOC removal) after 28 days (OECD, 2007; 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 diethanolamine. The K_{oc} for diethanolamine (as the charged molecule) was calculated to be 10 at pH values between 5 and 8 (Franco and Trapp, 2008; Franco et al., 2009; ECHA). [Kl. score = 2]

If released to water, based on its low K_{oc} and high water solubility values, diethanolamine is likely to remain in water and not adsorb to sediment. It is also not expected to adsorb to soil, and, has the potential to be highly mobile. However, the mobility of the substance is dependent on the cation exchange capacity of the soil (Government of Alberta, 2010)

E. . Bioaccumulation

There are no bioaccumulation studies on diethanolamine. The BCF was estimated to be 2.3 based on calculations from OASIS Catalogic v.5.11.15 [BCF base-line model v.0208] (Dimitrov et al., 2005; ECHA). Based on the log K_{ow} (-2.46) and the calculated BCF, bioaccumulation is not to be expected.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Diethanolamine exhibits moderate acute toxicity to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

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

Table 3 Acute Aquatic Toxicity Studies on Diethanolamine

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hour LC_{50}	460	2	ECHA
Pimephales promelas	96-hour LC_{50}	1,460*	2	Mayes et al. (1983)
Pimephales promelas	96-hour LC_{50}	1,664	2	ECHA
Lepomis macrochirus	48-hour LC_{50}	1,850	2	Turnbull et al. (1954)
Carassius auratus	24-hour LC_{50}	>5,000 (neutralised) 800 (non-neutralised)	2	Bridié et al. (1979)

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Ceriodaphnia dubia	48-hour EC_{50}	30.1 (24°C) 89.9 (20°C)	2	Cowgill et al. (1985)
Daphnia magna	48-hour EC_{50}	55	2	LeBlanc (1980)
Daphnia magna	48-hour EC_{50}	171	2	Zurita et al. (2005)
Pseudokirchneriella subcapitata	72-hour EC_{50} (growth rate)	9.5 (Test 1) 19 (Test 2)	2	ECHA
Desmodesmus subspicatus	72-hour EC_{50}	14.9 (growth rate) 6.2 (biomass)	2	ECHA
Desmodesmus subspicatus	72-hour EC_{50}	107.3 (growth rate) 74.5 (biomass)	2	ECHA
Chorella vulgaris	72-hour EC_{50}	778 (growth rate)	2	ECHA

*Geometric mean of 96-hour LC_{50} values of fry, juvenile and subadult fish. Not neutralised.

Chronic Studies

Table 4 lists the results of chronic aquatic toxicity studies on diethanolamine.

Table 4 Chronic Aquatic Toxicity Studies on Diethanolamine

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Daphnia magna	EC_{10} NOEC	1.05 0.76	1	ECHA
Pseudokirchneriella subcapitata	EC_{10} (growth rate)	1.4 (Test 1) 1.1 (Test 2)	2	ECHA
Desmodesmus subspicatus	EC_{10} (neutralised)	2.4 (growth rate) 2.0 (biomass)	2	ECHA
Desmodesmus subspicatus	EC_{10} (non-neutralised)	85.7 (growth rate) 41.3 (biomass)	2	ECHA
Pseudokirchneriella subcapitata	7-day NOEC	10	2	ECHA

C. Terrestrial Toxicity

In an earthworm (*Eisenia Andrei, Eisenia fetida*, or *Lumbricus terrestris*) study, the 35-day LC_{50} was 4,141 mg/kg soil dry weight (mortality); the 63-day EC_{50} was 776 mg/kg soil dry weight (reproduction); and the 63-day EC_{25} was 171 mg/kg soil dry weight (reproduction) (ECHA). [Kl. score = 2]

In a springtails (*Folsomia candida*) study, the 28-day LC_{50} was 8,301 mg/kg soil dry weight (mortality); the 28-day EC_{50} was 4,205 mg/kg soil dry weight (reproduction); and the 28-day EC_{25} was 2,102 mg/kg soil dry weight (reproduction) (ECHA). [Kl. score = 2]

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONERN

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).

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

The estimated BCF value for diethanolamine calculated from a QSAR model is 2.3; thus, it does not meet the criteria for bioaccumulation.

The EC_{10} or NOEC values from the chronic aquatic toxicity studies on diethanolamine are >0.1 mg/L. Thus, diethanolamine does not meet the screening criteria for toxicity. In a mouse dermal carcinogenicity study, there was an increased incidence of liver tumours in males and females and kidney tumours in males. However, both ECHA and NICNAS have concluded that "[t]he data on the mode of action are insufficient to conclude that diethanolamine-induced tumours in mice are relevant for humans and, therefore, based on the available information, diethanolamine is not classified for carcinogenicity." Thus, diethanolamine does not meet the criteria for toxicity.

Therefore, diethanolamine is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for diethanolamine

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]	
Diethanolamine	111-42-2	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

Bridié AL, Wolff CJM, and Winter M. (1979). The acute toxicity of some petrochemicals to goldfish. Water Research 13, 623-626.

Cowgill, U.M., Takahashi, I.T., and Applegath, S.L. (1985). A comparison of the effect of four benchmark chemicals on Daphnia magna and Ceriodaphnia dubia-affinis tested at two different temperatures. Environ. Toxicol. Chem. 4: 415-422.

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.

Dimitrov, S., Dimitrova, N., Parkerton, T., Comber, M., Bonnell, M., and Mekenyan, O. (2005). SAR and QSAR in Environ. Res. 16: 1-24.

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.

Franco, A., and Trapp, S. (2008). Estimation of the soil-water partition coefficient normalized to organic carbon for ionizable organic chemicals. Environ. Toxicol. Chem. 27: 1995-2004.

Franco, A., Fu, W., and Trapp, S. (2009). Influence of the soil on the sorption of ionizable chemicals: modeling advances. Environ. Toxicol. Chem. 28: 468-464.

Government of Alberta. 2010. Soil and Groundwater Remediation Guidelines for Monoethanolamine and Diethanolamine. December 2010.

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.

LeBlanc, G.A. (1980). Acute toxicity of priority pollutants to water flea (Daphnia magna). Bull. Environ. Contam. Toxicol. 24: 684-691.

Mayes, M.A., Alexander, H.C., and Dill, D.C. (1983). Study to assess the influence of age on the response of fathead minnows in static acute toxicity tests. Bull. Environ. Contam. Toxicol. 31: 139-147.

OECD. (2007). SIDS Initial Assessment Report for SIAM 24: 2,2'-Iminodiethanol (CAS No. 111-42-2).

Turnbull, H., DeMann, J.G., and Weston, R.F. (1954). Toxicity of various refinery materials to fresh water fish. Ind. Eng. Chem. 46: 324-333.

Zurita, J.L., Repetto, G., Jos. A., del Peso, A., Salguero, M., López-Artíguez, A., Olano, D., and Cameán, A. (2005). Ecotoxicological evaluation of diethanolamine using a battery of microbiotests. Toxicol. In Vitro 19: 879-886.

B. Abbreviations and Acronyms

^{o}C	degrees Celsius
^{o}F	degrees Fahrenheit
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
mg/kg	milligram per kilogram
mg/L	milligram per litre
mPa s	millipascal second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic

QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases