DIETHYLENE GLYCOL

This dossier on diethylene glycol presents the most critical studies pertinent to the risk assessment of diethylene glycol in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The 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 – Diethylene glycol is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Diethylene glycol is derived as a co-product with ethylene glycol (MEG) and triethylene glycol. The industry generally operates to maximize MEG production. Ethylene glycol is by far the largest volume of the glycol products in a variety of applications. Availability of diethylene glycol will depend on demand for derivatives of the primary product, ethylene glycol, rather than on diethylene glycol market requirements.

Diethylene glycol is readily biodegradable and unlikely to bioaccumulate. Diethylene glycol has low potential to adsorb to soil and sediment. Diethylene glycol is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

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

CAS RN: 111-46-6

Molecular formula: C_4H10O_3 or $(CH_2CH_2OH)_2O$

Molecular weight: 106.12 g/mol

Synonyms: Diethylene glycol; 2,2'-oxydiethanol; diglycol; bis(2-hydroxyethyl) ether; 2-hydroxyethyl ether; 2,2'-oxybisethanol; 2-(2-hydroxyethoxy)ethanol; ethanol, 2,2'-oxybis-; 2-(2-hydroxyethoxy)ethan-1-ol; glycol ethyl ether; ethylene diglycol.

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 Diethylene Glycol

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	A colorless viscous liquid	2	ECHA
Melting point	-6.5°C @ 101.3 kPa	2	ECHA
Boiling point	244.9°C @ 101.3 kPa	2	ECHA
Density	1,118 kg/m^3 @ 20°C	2	ECHA
Vapor pressure	0.008 hPa @ 25°C	2	ECHA
Partition coefficient (log K_{ow})	-1.98 (calculated)	2	ECHA
Water solubility	1,000 g/L @ 20°C	2	ECHA
Viscosity	30 mPa s (dynamic) @ 25°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 diethylene glycol.

NICNAS has assessed diethylene glycol in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment[1] .

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

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=111-46-6%2C+

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

The substance is readily biodegradable, is unlikely to bioaccumulate, nor is it likely to adsorb or desorb to soil or sediment to a great extent.

B. Biodegradation

Diethylene glycol is readily biodegradable. In an OECD 301B test, there was 70-80% and 90-100% degradation after 28 days, as determined by CO2 evolution and DOC removal respectively (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).

In an OECD 301A test, there was 90-100% degradation after 28 days, although the 10-day window was missed (ECHA) [Kl. score = 1]. In a modified MITI I test (OECD 301C), there was up to 92% degradation after 28 days (ECHA) [Kl. score = 2].

C. Environmental Distribution

No experimental data are available for diethylene glycol. Using KOCWIN in EPISUITE™ (USEPA, 2017), the estimated K_{oc} value from the molecular connectivity index (MCI) and log K_{oc} are 1 and -0.08 L/kg, respectively (ECHA) [Kl. Score = 2]. Based on these K_{oc} values, if released to soil, diethylene glycol is expected to not adsorb to soil and have a very high mobility. If released to water, based on the K_{oc} value and its water solubility, it is also not expected to adsorb to suspended solids and sediment.

D. Bioaccumulation

The calculated log Kow for diethylene glycol is -1.98 (Verschueren, 1983). Diethylene glycol has low potential to bioaccumulate. In a three-day bioaccumulation fish study with Leuciscus idus melanotus, the BCF was determined to be 100 (Freitag et al., 1985) [Kl. score = 2].

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

The substance is of low toxicity concern to aquatic organisms.

A. Aquatic Toxicity

Acute Studies

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

Table 3: Acute Aquatic Toxicity Studies on Diethylene Glycol

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pimephales promelas	96-h LC_{50}	75,200	2	ECHA
Oncorhynchus mykiss	96-h LC_5	66,000	2	ECHA

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Daphnia magna	24-h EC_{50}	>10,000	2	ECHA
Daphnia magna	48-h EC_{50}	65,980	2	ECHA
Daphnia magna	48-h EC_{50}	62,630	2	ECHA

Chronic Studies

In ECHA, the aquatic toxicity of the 'ethylene glycol and higher glycols' (mono-, di-, tri-, tetra- and pentaethylene glycol) is evaluated in a read-across approach. Data on all three trophic levels (fish, daphnia, algae) are available to describe the aquatic toxicity of the glycol read-across members. Due to the fact, that not for each single substance data for all required endpoints are available, a weight of evidence approach is used, which includes additional information based on QSAR calculation with the EpiWin-Program ECOSAR v1.11. Measured data as well as estimated data demonstrate, that all glycols within the read-across are not harmful to aquatic organisms. No adverse effects on aquatic organisms occurred up to concentrations above 100 mg/L (ECHA).

No data for fish was available for diethylene glycol. However, chronic studies for fish are available for ethylene glycol (CAS-No.: 107-21-1). The 7-day NOEC for the fathead minnow (*Pimephales promelas*) was determined to be 15,380 mg/L based on the weight of the test organisms (ECHA) [Kl. Score = 2].

No data for invertebrates was available for diethylene glycol. However, three studies were conducted with Dapnids (*Ceriodaphnia dubia* or *Daphnia magna*) for ethylene glycol (CAS-No.: 107-21-1) or triethylene glycol (CAS No.: 112-27-6). The study with ethylene glycol was conducted according to EPA guideline 600/4-89/001 with *Ceriodaphnia dubia* as test species. The 7-day NOEC for reproduction was determined to be 8,590 mg/L ethylene glycol (nominal). Two studies measured the effect of triethylene glycol on the reproduction of *Daphnia magna*. One study was conducted according to the national standard ASTM (E 47.01, Draft No. 1, "Draft proposed standard practice for conducting renewal life cycle toxicity tests with Daphnia magna"). In this test the Daphnids were exposed to triethylene glycol for 21 days. Based on reproduction the reported NOEC is > 15,000 mg/L triethylene glycol (nominal). (ECHA) [Kl. Score = 2].

Data for algae was available for diethylene glycol. The 8-day TGK to algae *Scenedesmus quadricauda* was determined to be 2,700 mg/L for diethylene glycol (ECHA) [Kl. score = 2].

From the QSAR calculations it can be expected for diethylene glycol that algae are slightly more sensitive (ChV = 1,200 mg/L) than invertebrates (ChV = 1,891 mg/L) or fishes (ChV = 7,694 mg/L). (ECHA) [Kl. Score = 2].

B. 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).

Diethylene glycol has been shown to be readily biodegradable; thus, it does not meet the screening criteria for persistence. The calculated log $K_{ow}$is -1.98, and the experimental BCF is 100. Thus, diethylene glycol does not meet the screening criteria for bioaccumulation.

The lowest chronic toxicity value for diethylene glycol is >0.1 mg/L. Thus, diethylene glycol does not meet the criteria for toxicity.

Therefore, diethylene glycol is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for diethylene glycol.

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]	
Diethylene glycol	111-46-6	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.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry

kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand