

ETHANOL, 2,2'-OXYBIS-, REACTION PRODUCTS WITH AMMONIA, MORPHOLINE DERIVATIVES RESIDUES

This dossier on ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues presents the most critical studies pertinent to the risk assessment in its use in hydraulic fracturing fluids and water treatment systems. 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 – Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues is a UVCB with several compounds containing ionizable groups. It does not biodegrade but is not expected to bioaccumulate based on its low log K_{ow} . It is of low aquatic toxicity concern and is not a PBT.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2-(2-hydroxyethoxy)ethan-1-ol; 2-[1-(morpholin-4-yl)ethoxy]ethan-1-amine; 2-{2-[bis(2-hydroxyethyl)amino]ethoxy}ethan-1-ol; 4-{2-[2-(morpholin-4-yl)ethoxy]ethyl}morpholine; morpholin-3-one

CAS RN: 68909-77-3

Molecular formula: $C_{36}H_{78}N_6O_{14}$

Molecular weight: 210.27 g/mol (Substance is a UVCB)

Synonyms: Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine product tower residues, Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivs. residues, Morpholine product tower residue.

3 PHYSICO-CHEMICAL PROPERTIES

The substance is defined as the residuum from the reaction of diethylene glycol and ammonia. It consists predominantly of morpholine-based derivatives such as [(aminoethoxy)ethyl]morpholine, [(hydroxyethoxy)ethyl]morpholine, 3-morpholinone, and 4,4'-(oxydi-2,1-ethanediyl)bis[morpholine].

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

Table 1 Overview of the Physico-Chemical Properties of ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	dark brown liquid	2	ECHA
Melting Point	-20 °C @ 101.3 kPa	1	ECHA
Boiling Point	223 °C @ 101.3 kPa	1	ECHA
Density	1090 kg/m ³ @ 20°C	1	ECHA
Vapour Pressure	0.55 Pa @ 25 °C	1	ECHA
Partition Coefficient (log K _{ow})	0.565 @ 20 °C and pH=7	1	ECHA
Water Solubility	100 g/L @ 25 °C	1	ECHA
Viscosity	121.398 mm ² /s (static) @ 20 °C ¹	1	ECHA
Dissociation constant (pKa at 20°C)	The test substance is a UVCB with several compounds containing ionizable groups a single pKa cannot be defined.	-	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 ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues.

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 Dynamic values in mPa s not available

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues is inherently biodegradable. It is not expected to bioaccumulate nor is it anticipated to sorb to soils or sediment due to its high water solubility and low log K_{ow} .

B. Partitioning

Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues is highly soluble in water. Based upon a Henry's Law constant of $1.02 \times 10^{-3} \text{ Pa}\cdot\text{m}^3/\text{mol}$, it is expected to have a low potential to volatilise from water and moist soil surfaces. However, it is expected to volatilise from dry soil surfaces based upon its vapour pressure. After evaporation or exposure to air, the substance will be rapidly degraded by photochemical processes (ECHA).

Hydrolysis is not expected. The assessment of hydrolytic stability of the substance was carried out according to the EU Method C.7. Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues was determined to be hydrolytically stable at pH 4, 7 and 9, with estimated half-lives greater than 1 year at 25°C (ECHA) [KI. Score = 1].

C. Biodegradation

Two key studies are available and used to conclude on the ready biodegradability of the substance in an aerobic aqueous medium. Both studies are given a Klimisch score of 1 and were conducted under GLP. The first study (Clarke, 2010 - report 41003975) is carried out according to the OECD guideline 301B (CO₂ evolution test), EC Method C.4-C. After 28 days, the observed biodegradation was 21% and the test substance is regarded as not readily biodegradable. The second study (Clarke, 2010 - report 41003980) is an enhanced biodegradation test carried out according to the OECD guideline 301B (CO₂ evolution test), EC Method C.4-C. After 28 days, the observed biodegradation was 15%, and after 42 days, the observed biodegradation was 18%. The test substance is regarded as not readily biodegradable [KI Score = 1](ECHA) but can be considered inherently biodegradable

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

D. Environmental Distribution

Adsorption/desorption studies were performed according to the EU Method C.19. The adsorption coefficient (K_{oc}) of Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues was determined to range from <17.8 (test material concentration of 89.6%) to 141 (test material concentration of 10.4%) at pH 5.5 and <17.8 (test material concentration of 89.6%) to 29.8 (test material concentration of 10.4%) at pH 7.5. The different K_{oc} values obtained at different pH values, might result from ionization. Overall, significant adsorption is not expected [KI Score = 1](ECHA).

Based upon these K_{oc} values, if released to soil, the substance is expected to have high mobility. If released into water, based on its high water solubility and these K_{oc} values, the substance is not expected to adsorb to suspended solids and sediment in water; and, as noted earlier, will dissociate.

E. Bioaccumulation

The substance has a low potential for bioaccumulation. Based on the available information on the log K_{ow} of the major components of the mixture "ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivs. residues" (CAS 68909-77-3) ranging from -2.26 to 0.5 (see IUCLID chapter 4.7) and supported by a weight-of-evidence approach from experimental and additional calculated data, it can be concluded that significant accumulation in organisms is not to be expected [KI Score = 1](ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivs. residues is of low acute toxicological concern to aquatic organisms. Details are provided below.

B. Aquatic Toxicity

Acute Studies

Table 3 presents the results of acute aquatic toxicity studies on ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues.

Table 3 Acute Aquatic Toxicity Studies on ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
<i>Oncorhynchus mykiss</i>	96-hr LC ₅₀	45	1	ECHA
<i>Daphnia magna</i>	48-hr EC ₅₀	100	1	ECHA
<i>Pseudokirchneriella subcapitata</i>	72-hr EC ₅₀	45	1	ECHA

Chronic Studies

No chronic studies are available. Chemical safety assessments have not indicated the need to investigate further the effects on fish or invertebrates. The acute-to-chronic ratio (ACR) as determined following the ECETOC Technical Report No. 93 (Aquatic Hazard Assessment II; ECETOC, 2003) shows that a long-term NOEC for fish of > 0.45 mg/L and for daphnids of > 1 mg/L is to be expected. Moreover, the results from short-term toxicity tests on fish, Daphnia and algae demonstrate that aquatic invertebrates are the most sensitive trophic level tested (ECHA) [KI. Score = 2].

C. Terrestrial Toxicity

No studies were found. The substance is not readily biodegradable. However, as the log K_{oc} of the mixture components is below 3, a low adsorption potential is indicated. Therefore, binding to

sewage sludge is unlikely and as a consequence a transfer to the soil compartment is not expected. Therefore, no tests on terrestrial organisms were provided (ECHA).

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).

Although ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues exhibits limited degradation, it is not readily biodegradable according to the specifics of degradation testing. However, it is considered inherently biodegradable...

Bioaccumulation of ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues is not expected to occur based on its low K_{ow} . Therefore, the substance does not meet the screening criteria for bioaccumulation.

There are no chronic aquatic toxicity data available on ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues. The acute E(L)C₅₀ values > 1 mg/L. Thus, ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine does not meet the criteria for toxicity.

The overall conclusion is that ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues.

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	
ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues	68909-77-3	Not a PBT	No	No	No ⁴	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.

4 - Substance is not readily biodegradable per testing guidelines. However, the degradation rate exhibited suggests it the substance is inherently biodegradable.

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.

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.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
CO ₂	Carbon dioxide
DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	Dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
g/mol	grams per mol
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m ³	kilogram per cubic metre
KI	Klimisch scoring system
kPa	kilopascal

L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
mPa s	millipascal second
NOEC	no observed effect concentration
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases