CHOLINE CHLORIDE

This dossier on choline chloride presents the most critical studies pertinent to the risk assessment of choline chloride 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 OECD-SIDS documents on choline chloride (OECD, 2004), and 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 – Choline chloride is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Choline chloride is readily biodegradable. Distribution modelling using Mackay Level 1 shows choline to be distributed completely into water. Choline chloride is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2-Hydroxy-N,N,N-trimethylethanaminium chloride

CAS RN: 67-48-1

Molecular formula: $C_5H_{14}NO.Cl$
$C_5H_{14}NO^+$ (choline)

Molecular weight: 139.6 g/mol
104.2 g/mol (choline)

Synonyms: Choline chloride; 2-hydroxy-N,N,N-trimethylethanaminium chloride; trimethyl(2-hydroxyethyl)ammonium chloride; cholinium chloride; 2-hydroxyethyl(trimethyl)azanium chloride

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 Choline Chloride

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa*	White crystalline solid*	2	OECD (2004)
Melting Point	~ 200°C @ 101.3 kPa	1	ECHA
Boiling Point	Decomposition at 305°C @ 101.3 kPa prior to boiling.	2	ECHA

Property	Value	Klimisch score	Reference
Density	70% aq. solution: 1110 kg/m^3@ 20°C	4	OECD (2004)
Vapour Pressure	2287.2 Pa @ 25°C (QSAR)	2	ECHA
Partition Coefficient (log K_{ow})	75% aq. solution: -3.77 @ 25°C	1	ECHA
Water Solubility	Powder containing 50% choline chloride: 650 g/L (temperature unknown)	4	OECD (2004)
Viscosity	75% aq. solution: 26.2 mPa.s @ 20°C; 14.1 mPa.s @ 40°C	1	ECHA

*Choline chloride is a white crystalline solid; it is marketed as an aqueous solution (70-75% w/w in water), which is colourless with an amine-like odour.

Choline chloride is a quaternary amine salt that will dissociate in water into choline ($C_5H_{14}NO^+$) and chloride (Cl^-) ions.

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 choline chloride.

Based on an assessment of environmental hazards, NICNAS identified cholide chloride as a chemical of low concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

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

Choline chloride is readily biodegradable. Distribution modelling using Mackay Level 1 shows choline to be distributed completely into water. Choline chloride will not adsorb on soil and sediments. It is not expected to bioaccumulate.

B. Partitioning

Choline chloride is highly water soluble and non-volatile. When released to water under typical environmental conditions, the quaternary ammonium salt dissociates to release a positively charged choline ion and a negatively charged chloride ion (OECD, 2004). It is unlikely to partition to the atmosphere based on its low volatility (OECD, 2004).

C. Biodegradation

Choline chloride is readily biodegradable (93% within 14 days) in a MITI-I test (MITI, 1992; OECD, 2004). In another MITI-I test, biodegradation was ≥60%, indicating ready biodegradation (Tunkel *et al.*, 2000; OECD, 2004). A $BOD_5/ThOD_5$ ratio of 75% was obtained in a BOD_5 test performed according to DIN 38409 part 43 (BASF AG, 1984; OECD, 2004). 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 choline. Choline is a quaternary ammonium compound (QAC); these compounds are not included in the training set for the K_{oc} estimation of the QSAR model KOCWIN v. 2.00 in EPISuite™ (USEPA, 2016), and therefore outside the program's prediction domain. A K_{oc} value of 2.3 had been estimated using the older QSAR model PCKOCWIN v. 1.66 (OECD, 2004), indicating a low potential for soil adsorption potential.

Results from Mackay Level I modelling indicate that choline chloride will be distributed completely into water (OECD, 2004).

E. Bioaccumulation

No measured data on bioaccumulation of choline chloride are available. An experimental log K_{ow} is -3.77, which indicates a low potential to accumulate in organisms (OECD, 2004). Bioaccumulation is not expected in aquatic organisms.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Choline chloride is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on choline chloride.

Table 3 Acute Aquatic Toxicity Studies on Choline Chloride

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oryzias latipes	96-hour LC_{50}	>100 (nominal and measured)	1	MOE Japan (1999a); OECD (2004)
Leuciscus idus	96-hour LC_{50}	>10,000*	2	OECD (2004); ECHA
Daphnia magna	48-hour EC_{50}	349 (nominal and measured)	2	MOE Japan (1999a); OECD (2004)
Daphnia magna	48-hour EC_{50}	>500*	2	OECD (2004)
Pseudokirchneriella subcapitata	72-hour EC_{50}	>1,000 (nominal and measured)	1	MOE Japan (1999a); OECD (2004)

*78% aqueous solution of choline chloride.

Chronic Studies

In a 21-day *Daphnia magna* reproduction test, the nominal and measured NOEC was reported to be 30.2 mg/L (MOE Japan, 1999d) [Kl. score = 1].

The NOEC from a 72-hour algae *Pseudokirchneriella subcapitata* study is 30.2 mg/L (MOE Japan, 1999c; OECD, 2004) [Kl. score = 1].

C. Terrestrial Toxicity

No data are available.

Choline is present in all plant and animal cells, mostly in the form of phospholipids (phosphotidylcholine or lecithin, lysophosphatidylcholine, choline plasmalogens and sphingomyelin), which are essential components of membranes (IOM, 2000).

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).

Choline chloride is readily biodegradable and thus it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of -3.77, choline chloride does not meet the criteria for bioaccumulation.

The NOEC values from chronic toxicity studies on choline chloride are >0.1 mg/L. Thus, choline chloride does not meet the criteria for toxicity.

The overall conclusion is that choline chloride is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for choline chloride.

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]	
Choline Chloride	67-48-1	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

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BOD	biological oxygen demand
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
DIN	Deutsches Institut für Normung
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
HENRYWIN	EPISuite modelling component to calculate the Henry's Law constant
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre

KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
m^3	cubic metre
mg/L	milligrams per litre
MITI	Japanese Ministry of International Trade and Industry
mPas	millipascal second
OECD	Organisation for Economic Co-operation and Development
Pa m^3/mol	pascal meter squared per gram molecular weight
PBT	Persistent, Bioaccumulative and Toxic
PCKOCWIN	USEPA Episuite modelling component to calculate K_{oc}
QAC	quaternary ammonium compound
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	Screening Information Data Set
ThOD	theoretical oxygen demand