

## ALCOHOLS, C12-15, ETHOXYLATED

This dossier on alcohols, C12-15, ethoxylated presents the most critical studies pertinent to the risk assessment of alcohols, C12-15, ethoxylated in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the Human & Environmental Risk Assessment on Ingredients of European Household Cleaning Products: Alcohol Ethoxylates (HERA, 2009), and 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 – Alcohols, C12-15, ethoxylated is classified as a **tier 1** chemical and requires a hazard assessment only.

### 1 BACKGROUND

Alcohol ethoxylates (AE) are a class of non-ionic surfactants that have the basic structure  $C_{x-y}AE_n$ . The subscript (x-y) following the 'C' indicates the range of carbon chain units. The hydrocarbon chain can be either linear or branched. AEs also contain an ethylene oxide (E) chain attached to the alcohol. The degree of ethylene oxide polymerisation is indicated by the subscript (n) which indicates the average number of ethylene oxide units. Alcohols, C12-15, ethoxylated (CAS No. 68131-39-5) has an average number of 1 to 2.5 moles of ethylene oxide units.

Alcohols, C12-15, ethoxylated are readily biodegradable, are not likely to sorb to sediments or soil, have low potential to bioaccumulate or bioconcentrate and are of low toxicity to environmental receptors.

### 2 CHEMICAL NAME AND IDENTIFICATION

**Chemical Name (IUPAC):** Alcohols, C12-15, ethoxylated

**CAS RN:** 68131-39-5

**Molecular formula:**  $(C_2H_4O)_{1-3}(CH_2)_{10-13}C_2H_6O$

**Molecular weight:** Not available

**Synonyms:** Alcohols, C12-15, ethoxylated

### 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 Alcohols, C12-15, Ethoxylated (1 to 2.5 moles ethoxylated)**

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Clear liquid with a rancid odour*	2	ECHA
Melting Point	7.22°C (pressure not provided)	2	ECHA
Boiling Point	ca. 287°C @ 101.3 kPa	1	ECHA
Density	926 kg/m <sup>3</sup> @ 15.56°C	1	ECHA
Vapour Pressure	Negligible	-	ECHA
Partition coefficient (log K <sub>ow</sub> )	5.06* @ 25°C	2	ECHA
Water Solubility	0.007 – 0.063 g/L @ 25°C	2	ECHA
Dissociation constant (pKa)	No dissociation	-	ECHA
Viscosity	28.1 mPa s (dynamic) @ 20°C	2	ECHA

\*Based on alcohols, C12-14, ethoxylated (1 to 2.5 EO) [CAS No. 68439-50-9]

#### 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 alcohols, C12-15, ethoxylated.

**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

Alcohols, C12-15, ethoxylated is readily biodegradable. It has a low potential for bioaccumulation and a moderate potential for adsorption to soil and sediment.

## B. Biodegradation

Alcohols, C12-15, ethoxylated is readily biodegradable. In an OECD 301B test, degradation was 72% in 28 days, but failed the 10-day window (ECHA) [KI. score = 1].

An alcohol, C12-15, ethoxylated (7 EO) degraded 80 to 88% in 28 days when tested using a shake-flask CO<sub>2</sub>-evolution test method (ECHA) [KI. 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).

## C. Environmental Distribution

No experimental data are available for alcohols, C12-15, ethoxylated. Using KOCWIN in EPISuite™ (USEPA, 2018), the estimated K<sub>oc</sub> values for surrogates of alcohols, C12-15, ethoxylated are:

C12 linear alcohol, ethoxylated (2 EO): 279.5 L/kg (MCI) and 464.2 L/kg (K<sub>ow</sub>)

C15 linear alcohol, ethoxylated (2 EO): 1,691 L/kg (MCI) and 3,018 L/kg (K<sub>ow</sub>)

Based on these values, the substance has a moderate potential for adsorption to soil or sediments and a low potential for mobility.

## D. Bioaccumulation

The potential for bioaccumulation of alcohol ethoxylates is considered low due to the biotransformation and excretion of the substance. The BCF values for alcohol ethoxylates in fathead minnows have been reported to range from <5 to 387.5 (Toll et al., 2000). The uptake rates varied from 330 to 1660 (L x kg/day) and elimination rates varied from 3.3 to 59 per day (Toll et al., 2000). The high concentrations in fish is thought to be prevented by an efficient biotransformation of the alcohol ethoxylates, leading to a high elimination rate.

# 6 ENVIRONMENTAL EFFECTS SUMMARY

## A. Summary

Alcohol, C12-15, ethoxylated has moderate chronic toxicity concern to aquatic life.

## B. Aquatic Toxicity

In developing a water quality guideline for alcohol ethoxylates (ANZG, 2018), the toxicity data was normalised for a specific alkyl chain length or a specific number of ethoxylate (EO) groups. The NOECs listed below were normalised to an alkyl chain length of C13.3 and EO of 8.2.

Freshwater fish: 2 species, 720 to 1,500 mg/L.

Freshwater crustaceans: 2 species, 590 to 860 mg/L.

Freshwater rotifers: 1 species, *Brachionus calyciflorus*, 1,300 mg/L

Freshwater algae, diatoms and blue-green algae: 6 species, 200 to 8,700 mg/L.

Freshwater mesocosms: 4 NOEC data for multiple species tests were 80, 80, 320 and 330 mg/L, although replication was insufficient to meet OECD (1992) requirements. Normalised data were 380, 380, 320 and 1,520 mg/L.

### **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).

Alcohols, C12-15, ethoxylated is readily biodegradable and thus does not meet the screening criteria for persistence.

The bioconcentration factors (BCF) in fish for ethoxylated alcohols (which includes alcohols, C12-15, ethoxylated) have been reported to range from <5 to 387.5. Thus, alcohols, C12-15, ethoxylated does not meet the screening criteria for bioaccumulation.

The chronic NOEC values for alcohols ethoxylates are >0.1 mg/L. Thus, alcohols, C12-15, ethoxylated do not meet the criteria for toxicity.

Thus, alcohols, C12-15, ethoxylated is not a PBT substance.

### **B. Other Characteristics of Concern**

No other characteristics of concern were identified for alcohols, C12-15, ethoxylated.

## 8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment <sup>1</sup>	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required <sup>3</sup>
			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 <sup>2</sup>	Chronic Toxicity <sup>2</sup>	
Alcohols, C12-15, ethoxylated	68131-39-5	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

ANZG. 2018. Australian and New Zealand Guidelines for Fresh and Marine Water Quality. Australian and New Zealand Governments and Australian state and territory governments, Canberra ACT, Australia. Available at [www.waterquality.gov.au/anz-guidelines](http://www.waterquality.gov.au/anz-guidelines)

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: <https://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.

Human and Environmental Risk Assessment (HERA) on Ingredients of Household Cleaning Products: Alcohol Ethoxylates (2009). <https://www.heraproject.com/>

OECD. (1992). Report of the OECD workshop on extrapolation of laboratory aquatic toxicity data to the real environment. OECD Environment Monographs No. 59, Organisation for Economic Co-operation and Development, Paris.

Toll, J., Haller, M., Labee, E., Verweij, M., and Sijm, D.T.H.M. (2000). Toxicology and Chemistry, 19 646–653.

USEPA. (2018). 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
AE	alcohol ethoxylates
AICS	Australian Inventory of Chemical Substances
ANZG	Australian and New Zealand Government
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EO	ethoxylate
EU	European Union
g/l	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/mg <sup>3</sup>	kilograms per cubic metre
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
MCI	molecular connectivity index
mg/L	milligrams per litre
mPA s	millipascal second
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases