

BUTYL ALCOHOL (1-BUTANOL)

This dossier on butyl alcohol (1-butanol) presents the most critical studies pertinent to the risk assessment of 1-butanol 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 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; KI).

Screening Assessment Conclusion – Butyl alcohol is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

n-Butanol or n-butyl alcohol or normal butanol is a primary alcohol with a 4-carbon structure and the chemical formula C_4H_9OH . Its isomers include isobutanol, 2-butanol and tert-butanol. Butanol is one of the group of "fusel alcohols" which have more than two carbon atoms and have significant solubility in water. n-Butanol occurs naturally as a minor product of the fermentation of sugars and other carbohydrates, and is present in many foods and beverages. It is also a permitted artificial flavorant in the United States, used in butter, cream, fruit, rum, whiskey, ice cream and ices, candy, baked goods and cordials. It is also used in a wide range of consumer products.

The largest use of n-butanol is as an industrial intermediate, particularly for the manufacture of butyl acetate (itself an artificial flavorant and industrial solvent). It is a petrochemical, manufactured from propylene and usually used close to the point of manufacture.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Butan-1-ol

CAS RN: 71-36-3

Molecular formula: $C_4H_{10}O$

Molecular weight: 74.123 g/mol

Synonyms: 1-Butanol, 1-Butyl alcohol, 1-hydroxybutane, Butan-1-ol, butyl alcohol, Butyl hydroxide, Butylalcohol, CCS 203, ET5740PTB, Hemostyp, Methylolpropane, n-Butanol, n-Butyl alcohol, N300PTB, Nacol 4, PP100, Propylcarbinol

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 1-Butanol

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Clear, colourless liquid with an alcoholic odour	-	PubChem
Melting point	<-90°C (pressure not provided)		PubChem
Boiling point	117°C (pressure not provided)		PubChem
Density	810 kg/m ³ @ 20°C		PubChem
Vapour pressure	< 1000 Pa @20°C		PubChem
Partition coefficient (log K _{ow})	1 @ 25°C		PubChem
Water solubility	66 g/L @ 20°C		PubChem
Dissociation Constant (pKa)	16.1 @ 25°C	-	PubChem

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 butyl alcohol.

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

1-Butanol is readily biodegradable. It is not expected to bioaccumulate and has a low potential for adsorption to soil and sediment.

B. Partitioning

1-Butanol is highly soluble in water. Based upon a Henry's Law constant of 0.893 Pa*m³/mol, it is expected to volatilise from water and moist soil surfaces. It is also expected to volatilise from dry soil surfaces based upon its vapour pressure. Vapour-phase 1-butanol will be degraded in the

atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 45 hours (PubChem).

C. Biodegradation

1-Butanol is readily biodegradable. In a BOD test, degradation was 87% after 10 days and 92% after 20 days, meeting the 10-day window (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 1-butanol. Using KOCWIN in EPISuite™ (USEPA, 2019), the estimated K_{oc} value from $\log K_{ow}$ of 1.0 is 10.01 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 3.471 L/kg. Based upon these K_{oc} values, if released to soil, 1-butanol is expected to have very high mobility. If released into water, 1-butanol is not expected to adsorb to suspended solids and sediment in water; and, as noted earlier, volatilisation is expected to be an important fate process (PubChem).

E. Bioaccumulation

There are no bioaccumulation studies on 1-butanol. 1-Butanol is not expected to bioaccumulate based on a $\log K_{ow}$ of 1.0 (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

The substance exhibits a low order of acute and chronic aquatic toxicity as demonstrated by the information provided below.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on 1-butanol.

Table 3 Acute Aquatic Toxicity Studies on 1-Butanol

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
<i>Pimephelas promelas</i>	96-hour LC_{50}	1,376	1	ECHA
<i>Daphnia magna</i>	48-hour EC_{50}	1,328	1	ECHA
<i>Pseudokirchneriella subcapitata</i>	72-hour EC_{50}	225	1	ECHA

Chronic Studies

The 21-day NOEC from a *Daphnia* reproduction test is 4.1 mg/L (ECHA) [Kl. score = 2].

96-hour EC₁₀ to *Pseudokirchneriella subcapitata* is 134 mg/L (ECHA) [Kl. score = 1].

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).

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

Based on a measured log K_{ow} of 1.0, 1-butanol does not meet the screening criteria for bioaccumulation.

The lowest chronic EC₁₀ or NOEC value for 1-butanol is >0.1 mg/L. The acute EC₅₀ values are >1 mg/L. Thus, 1-butanol does not meet the criteria for toxicity.

The overall conclusion is that 1-butanol is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for butyl alcohol.

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	
Butyl Alcohol	71-36-3	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.

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.

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USEPA. (2019). 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
AICS	Australian Inventory of Chemical Substances
BOD	biological oxygen demand
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre

hPa	hectopascal
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
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