Hexanedinitrile

This dossier on hexanedinitrile presents the most critical studies pertinent to the risk assessment of hexanedinitrile in its use in drilling muds. Sufficient data does not exist for this particular substance. 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 National Industrial Chemicals Notification and Assessment Scheme (NICNAS, 1994) and the ECHA database that provides information on chemicals that have been registered under the European Union (EU) REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

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

1 BACKGROUND

Hexanedinitrile, also known as adiponitrile, is used as a clay inhibitor. It is readily biodegradable and has low potential to bioaccumulate or to absorb to soil. Hexanedinitrile is of low acute toxicity concern to aquatic life. Chronic aquatic toxicity studies were not available.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Hexanedinitrile

CAS RN: 111-69-3

Molecular formula: $C_6H_8N_2$

Molecular weight: 108.14 g/mol

Synonyms: 1,4-Dicyanobutane, adipodinitrile

3 PHYSICAL AND CHEMICAL PROPERTIES

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

Table 1 Overview of Physico-Chemical Properties of Hexanedinitrile

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Slightly brown liquid	1	ECHA
Melting Point	-5 °C to 6°C[1]	1	ECHA
Boiling Point	305.3°C @ 99.5 kPa	1	ECHA
Density	968 Kg/m^3@ 20°C	2	ECHA
Vapour Pressure	0.091 Pa @ 25°C	2	ECHA
Partition Coefficient (log K_{ow})	-0.32 @ 25°C	2	ECHA
Water Solubility	80 g/L @ 20°C	2	ECHA

[1] No information on the atmospheric pressure reported.

Property	Value	Klimisch score	Reference
Viscosity	58 mPa s @30°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 hexanedinitrile.

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

Hexanedinitrile is expected to readily degrade. It is not expected to bioaccumulate, and it has a low potential to adsorb to soil.

B. Partitioning

Hexanedinitrile is highly soluble in water. Volatilisation from water surfaces or moist soil surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. It is also not expected to volatilise from dry soil surfaces based upon its vapor pressure (Pub Chem).

C. Biodegradation

A closed bottle test was conducted according to OECD 301 (2009) and the result was noted as inherently biodegradable (ECHA) (KI Score = 2). No specific data on degradation rates were provided.

Another test was conducted according to OECD 301A (2002) and the result was noted as rapidly biodegradable (ECHA) (KI Score=1). No specific data on degradation rates were provided.

Based on the summarized data above, the USEPA EPISuite BIOWIN7 (Anaerobic Linear Model) was used to estimate the probability of ready biodegradability. The results of the modelling indicated that the substance has a high probability (0.94) of ready biodegradation.

Therefore, the weight of evidence suggests that the substance in readily degradable.

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

D. Environmental Distribution

No data were available on the adsorption/desorption properties of the substance.

Based on the lack of data for this parameter, USEPA EPISuite KOCWIN v2.00 was used to estimate the log K_{oc} of 1.305 using the molecular connectivity index (MCI) methodology. Based on this estimated value, hexanedintrile is expected to have very high mobility in soil. If released to water, based on the log K_{oc} value and its high water solubility, it is also not expected to adsorb to suspended solids and sediment.

E. Bioaccumulation

No data are available for the substance. Based on the lack of data available, USEPA EPISuite BCFBAF v 3.01 was used to estimate bioaccumulation based on the above noted log K_{ow} of -0.32 (Table 1). The modelled log bioconcentration factor (BCF) is equal to 0.5. Overall, the substance is not expected to bioaccumulate to a substantial degree based on the low log K_{ow} and predicted low log BCF.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Hexanedinitrile is of low acute toxicity potential to aquatic organism.

B. Aquatic Toxicity

Table 3 lists the results of acute aquatic toxicity studies on hexanedinitrile. It is expected to be readily biodegradable and is not expected to bioaccumulate.

Table 3 Acute Aquatic Toxicity Studies Hexanedinitrile

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Freshwater Fish[a]	96-hr LC_{50}	670	-	ECHA
Freshwater invertebrates[a]	48-hr EC_{50}	1189	-	ECHA
Pseudokirchneriella subcapitata	72-hr EC_{50} NOEC	>97.4	1	ECHA

a – Species not provided in study summary

No chronic studies were available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

Hexanedinitrile is readily biodegradable in the aquatic environment; thus, it does not meet the screening criteria for persistence.

The measured log K_{ow} for the substance is -0.32. Based on the calculated bioaccumulation factor of 0.5, hexanedinitrile is not bioaccumulative.

Acute toxicity for aquatic receptors across three tropic levels is > 1mg/L. Therefore, the substance does not fulfill the toxicity criterion.

The overall conclusion is that hexanedinitrile is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for hexanedinitrile.

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]	
Hexanedinitrile	111-69-3	Not a PBT	No	No	No	No	No	No	1	No data	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:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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.

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.

NICNAS. (1994). National Industrial Chemicals Notification and Assessment Scheme (NICNAS), AGPS, Canberra, Australia.

PubChem. National Institutes of Health. National Library of Medicine National Center for Biotechnology Information. https://pubchem.ncbi.nlm.nih.gov/

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
atm-cu m/mole	
BCF	bioconcentration factor
COC	constituent of concern
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
g/mL	grams per millilitre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal

LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
mm	millimetre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOEC	no observed effective 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
USEPA	United States Environmental Protection Agency