Fatty acids, tall-oil, reaction products with diethylenetriamine

This dossier on fatty acids, tall-oil, reaction products with diethylenetriamine presents the most critical studies pertinent to the risk assessment of fatty acids, tall-oil, reaction products with diethylenetriamine in its use in drilling muds, hydraulic fracturing fluids and water treatment. No sufficient data 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 – Fatty acids, tall-oil, reaction products with diethylenetriamine is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Fatty acids, tall-oil, reaction products with diethylenetriamine is considered a UVCB substance (substance of unknown or variable composition, complex reaction products or biological materials). It is expected to biodegrade over time. Based on a read-across to similar substance, adsorption to sediment and soils is expected to be substantial. Fatty acids, tall-oil, reaction products with diethylenetriamine are not expected to substantially bioaccumulate or bioconcentrate and the substance is of low toxicity concern to environmental receptors.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): fatty acids, tall-oil, reaction products with diethylenetriamine

CAS RN: 61790-69-0

Molecular formula: Not applicable as substance is a UVCB

Molecular weight: Variable

Synonyms: None

3 PHYSICAL AND CHEMICAL PROPERTIES

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

Table 1 Overview of the Physico-Chemical Properties of Fatty acids, tall-oil, reaction products with diethylenetriamine

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa*	Brown beige solid	1	ECHA
Melting Point	Shows a melting area of crystalline subcomponents at a temperature of 29°C; a glass transition temperature (Tg;	1	ECHA

Property	Value	Klimisch score	Reference
	amorphous components) was detected at ca. -55°C and ca. -51°C		
Boiling Point	117°C @ 101.3 kPa	1	ECHA
Density	970 kg/m^3 @ 20°C	1	ECHA
Vapour Pressure	1600 Pa @ 20°C	1	ECHA
Partition Coefficient (log K_{ow})	6 @ 20°C	1	ECHA
Water Solubility	0.0006 g/L @ 20°C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). 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 fatty acids, tall-oil, reaction products with diethylenetriamine.

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

Fatty acids, tall-oil, reaction products with diethylenetriamine are expected to biodegrade over time. Based on a read-across to similar substance, adsorption to sediment and soils is expected to be substantial. Fatty acids, tall-oil, reaction products with diethylenetriamine are not expected to substantially bioaccumulate or bioconcentrate and the substance is of low toxicity concern to environmental receptors.

B. Biodegradation

Two biodegradation tests were performed. A first test was performed according to OECD 301 B test criteria over 28 days. After 28 days the degradation reached 21% without reaching the plateau. In a second test, the degradation of the test item was tested in an extended OECD 301 B test for 60 days. On day 28 the degradation extent was 31 ±14% (mean ±SD). The degradation extent at the end of the test 60-day period was 65%.

Therefore, test item can be evaluated as inherently biodegradable under enhanced test conditions in this carbon dioxide evolution test based on the quantitative determination of the formed carbon dioxide in the test substance assays.

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

C. Environmental Distribution

No data are available for the substance. As an alternative, data were abstracted from the ECHA data base for eaction products of tall-oil fatty acids with diethylenetriamine and maleic anhydride: (CAS RN 1419212-76-2). The K_{oc} of a representative structure was calculated based a log K_{ow} of 6.5 and 11 (last value outside the applicability domain of the quantitative model). The test substance is a UVCB. Standard tests for this endpoint are intended for single substances and are not appropriate for this complex substance. Therefore, for risk assessment the log K_{oc} was set at 6.0 (ECHA) [KI Score = 3], indicating a strong potential for adsorption to soil and no mobility.

D. Bioaccumulation

No data are available for the substance. As an alternative, data were abstracted from the ECHA data base for reaction products of tall-oil fatty acids with diethylenetriamine and maleic anhydride: (CAS RN 1419212-76-2). The calculated log K_{ow} for the bioaccumulation of the surrogate test substance is based on a log K_{ow} of 6.5 is 2.58 (BCF 381.4). As the log K_{ow} of the surrogate is reasonably close to that of fatty acids, tall-oil, reaction products with diethylenetriamine (i.e., the dossier substance), the BCF of 381.4 is believed to be sufficient for risk assessment purposes. Based on this BCF, the substance is not expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Fatty acids, tall-oil, reaction products with diethylenetriamine are of low to moderate toxicity concern to environmental receptors.

B. Aquatic Toxicity

Table 2 lists the results of acute aquatic toxicity studies on salts of fatty acids, tall-oil, reaction products with diethylenetriamine.

Table 3 Acute Aquatic Toxicity Studies on Salts of fatty acids, tall-oil, reaction products with diethylenetriamine

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rerio	96-hr LC_{50}	11	1	ECHA
Daphnia magna	48-hr EC_{50}	10.4	1	ECHA
Pseudokirchneriella subcapitata	96-hr EC_{50} NOEC	10	1	ECHA

No chronic studies were available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

Fatty acids, tall-oil, reaction products with diethylenetriamine are inherently biodegradable in the aquatic environment; thus, it does not meet the screening criteria for persistence.

The measured log K_{ow} for fatty acids, tall-oil, reaction products with diethylenetriamine is 6. The calculated logK_{ow} for the bioaccumulation of the test substance based on a log K_{ow} of 6.5 is 2.58 (BCF 381.4). The substance fulfils the bioaccumulation criterion when BCF > 2000. Based on the calculated value, fatty acids, tall-oil, reaction products with diethylenetriamine are not bioaccumulative.

Acute toxicity for aquatic receptors across three tropic levels is > 10 mg/L. Therefore, tall-oil, reaction products with diethylenetriamine does not fulfill the toxicity criterion.

The overall conclusion is that fatty acids, tall-oil, reaction products with diethylenetriamine is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for fatty acids, tall-oil, reaction products with diethylenetriamine.

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]	
Fatty acids, tall-oil, reaction products with diethylenetriamine	61790-69-0	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.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
Atm	Atmosphere
BCF	bioconcentration factor
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
Kl	Klimisch scoring system
kPa	kilopascal
LC	lethal concentration
mbar	millibar
mg/L	milligrams per litre
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals

SD	Sprague Dawley
SGG	Synthetic Greenhouse Gases
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials