

FATTY ACIDS, TALL-OIL, ETHOXYLATED

This dossier on fatty acids, tall-oil, ethoxylated (FAT) presents the most critical studies pertinent to the risk assessment of the substance 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 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 – Fatty acids, tall-oil, ethoxylated is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

FAT is a UVCB used to facilitate emulsification. This CAS RN is broadly defined as a complex combination of hydrocarbons obtained by treating a petroleum fraction with hydrogen in the presence of a catalyst. Tall oil fatty acids (TOFA), generally any product containing 90% or more fatty acids and 10% or less of rosin, have grown in annual volume ever since, until they amounted to 398.8 million pounds annual production in the United States in 1978. Crude tall oil is a byproduct of the Kraft process for producing wood pulp from pine wood. Crude tall oil is about 50% fatty acids and 40% rosin acids, the remainder unsaps and residues. Separative and upgrading technology involves: (a) recovery of the tall oil; (b) acid refining; (c) fractionation of tall oil; and occasionally (d) conversion to derivatives. TOFA of good quality and colour of Gardner 2 corresponds to above 97% fatty acids with the composition of 1.6% palmitic and stearic acid, 49.3% oleic acid, 45.1% linoleic acid, 1.1% miscellaneous acids, 1.2% rosin acids and 1.7% unsaponifiables.

The substance is biodegradable, may sorb to sediments, is not expected to bioaccumulate and is of low toxicity to environmental receptors.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Fatty acids, tall-oil, ethoxylated

CAS RN: 61791-00-2

Molecular formula: C₍₁₈₋₅₀₎H₍₃₄₋₉₈₎O₍₃₋₈₎ (UVCB substance)

Molecular weight: (UVCB substance)

Synonyms: 2-[(10Z,13Z)-nonadeca-10,13-dienoyloxy]ethyl (10Z,13Z)-nonadeca-10,13-dienoate 2-hydroxyethyl (5Z,9Z,12Z)-octadeca-5,9,12-trienoate 2-hydroxyethyl (9Z)-octadec-9-enoate 2-hydroxyethyl (9Z,12Z)-octadeca-9,12-dienoate

3 PHYSICO-CHEMICAL PROPERTIES

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

Table 1 Overview of the Physico-chemical Fatty acids, tall-oil, ethoxylated

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Liquid.	2	ECHA
Melting point	-85°C @ 101.3 kPa	2	ECHA
Boiling point	Not available. During the heating process the test item began to change its state at approximately 172°C from liquid to highly viscous. This indicates a thermally caused change of the test item.	2	ECHA
Density	958 kg/m ³ @ 20°C	2	ECHA
Vapour pressure	The vapour pressure could not be determined.	2	ECHA
Partition coefficient (log K _{ow})	5.94 @ 25°C	-	-
Water solubility	The test item can be mixed with water up to a ratio of 3:7 (m (test item):m (water)).	-	-
Viscosity	58.0 mPa.s @ 20°C	2	ECHA

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 fatty acids, tall-oil, 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

There are no biodegradation data on FAT. However, data on structurally similar substances suggest FAT is biodegradable with potential to sorb to soils. It is not expected to readily bioaccumulate.

B. Biodegradation

Data on the ready biodegradability of fatty acids, tall oil, ethoxylated (> 1 < 2.5) (CAS 61791-00-2) are not available. Therefore, data on the ready biodegradability of the structurally related analogue substance fatty acids, tall oil, ethoxylated (EO 5) (CAS No. 9004-96-0) is used as read-across in accordance with Regulation (EC) No. 1907/2006, Annex XI, 1.5.

This read-across is justified because both target and source substance are structurally identical (ethoxylated oleic acid) except for the fact that the source substance is slightly higher ethoxylated (5 EO) than the target substance (1-2.5 EO). This difference might lead to a slightly lower water solubility of the target substance; however, since the solubility of both substances is rather high and not limiting the bioaccessibility of the substances to aquatic microorganisms, is not considered to influence the identical biodegradation behaviour of both substances. Both substances share the same functional groups and the same mode of action (baseline toxicity caused by the long lipophilic fatty acid chain). Thus, biotransformation can, with very high certainty, be assumed to be identical.

The test with the source substance was conducted according to OECD Guideline 301B, under GLP conditions (ECHA). Domestic, non-adapted activated sludge was exposed to the test substance for 28 days at 22°C, and biodegradation was measured by CO₂ consumption. After 28 days, the test substance reached a biodegradation of 90 - 100%.

Based on the results for the read-across substance, fatty acids, tall oil, ethoxylated (EO > 1 < 2.5) (CAS 61791-00-2) is considered to be readily biodegradable. 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

One study investigating the adsorption/desorption behaviour of fatty acids, tall-oil, ethoxylated (CAS 61791-00-2) is available. The study was performed according to GLP and OECD guideline 121 (ECHA). Six different peaks were observed with log K_{oc} values ranging from < 1.8 to > 5.63. The two main components (> 85%) show log K_{oc} values > 4. Thus, the substance shows moderate capacity to sorb to sediments.

Thus, adsorption of fatty acids, tall-oil, ethoxylated to solid soil is expected with limited potential for mobility.

D. Bioaccumulation

The test substance consists of components with log K_{ow} values in the range of 5 to > 10 (KOWWIN v1.68) indicating a potential for bioaccumulation. However, due to rapid environmental biodegradation, metabolisation via enzymatic hydrolysis (monoesters and diesters) as well as sterical hindrance of crossing biological membranes (high molecular weight of diesters) a relevant uptake

and bioaccumulation in aquatic organisms is not expected. This is supported by low BCF values of < 100 L/kg wet weight (BCFBAF v3.01, Arnot-Gobas, including biotransformation, upper trophic) calculated for different components of the UVCB (mono- and diester EO1 to EO5). Thus, taking all information into account, the test substance is not considered to be bioaccumulative.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

The substance is of low acute toxicity concern to aquatic life.

B. Aquatic Toxicity

Acute Studies

There are no aquatic toxicity data on the substance are listed on Table 3.

Table 3 Acute Aquatic Toxicity Studies on Fatty acids, tall-oil, ethoxylated*

Test Substance	Test Species	Endpoint	Results (mg/L) [WAF]	Kl. score	Reference
Fatty acids, tall-oil, ethoxylated	<i>Danio rerio</i>	96-hour LL ₅₀	>100	1	ECHA
Fatty acids, tall-oil, ethoxylated	<i>Daphnia magna</i>	48-hour LL ₅₀	12.41	1	ECHA
Fatty acids, tall-oil, ethoxylated	<i>Pseudokirchnerella subcapitata</i>	72-hour LL ₅₀	39.7	1	ECHA

*All studies used the water accommodated fractions (WAFs) of the test substance.

Chronic Studies

No chronic data were available

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).

FAT was noted to be readily biodegradable. Thus, the substance is not expected to meet the screening criteria for persistence.

Modelling of a representative structure indicates FAT does not have the potential to bioaccumulate. Thus, FAT does not meet the screening criteria for bioaccumulation.

FAT did not exhibit substantial acute toxicity to fish, invertebrates or algae. Thus, FAT is not expected to meet the screening criteria for toxicity.

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

B. Other Characteristics of Concern

No other characteristics of concern were identified for fatty acids, tall-oil, ethoxylated.

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, ethoxylated	61791-00-2	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.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
BCFBAF	USEPA EPISuite module to estimate bioconcentration and bioaccumulation factors
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	European Commission
ECHA	European Chemicals Agency
EU	European Union
FAT	fatty acids, tall-oil, ethoxylated
g/L	grams per litre
GLP	good laboratory practice
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m ³	kilogram per cubic metre

KOWWIN	USEPA program to estimate the organic carbon-normalised sorption coefficient for soil and sediment
kPa	kilopascal
L/kg	litres per kilogram
LL	Loading level
mg/L	milligram per litre
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
TOFA	tall oil fatty acid
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials
WAF	water accommodated fraction