6:2 Fluorotelomer sulfonate derivatives: Human health tier II assessment

12 December 2019

Chemicals in this assessment

Chemical Name in the Inventory	CAS Number
1-Propanaminium, N-(carboxymethyl)-N,N-dimethyl-3-[[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulfonyl]amino]-, hydroxide, inner salt	34455-29-3
Forafac 1157	65256-46-4
1-Propanaminium, N,N,N-trimethyl-3-[[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulfonyl]amino]-, iodide	94088-80-9

Preface

This assessment was carried out by staff of the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) using the Inventory Multi-tiered Assessment and Prioritisation (IMAP) framework.

The IMAP framework addresses the human health and environmental impacts of previously unassessed industrial chemicals listed on the Australian Inventory of Chemical Substances (the Inventory).

The framework was developed with significant input from stakeholders and provides a more rapid, flexible and transparent approach for the assessment of chemicals listed on the Inventory.

Stage One of the implementation of this framework, which lasted four years from 1 July 2012, examined 3000 chemicals meeting characteristics identified by stakeholders as needing priority assessment. This included chemicals for which NICNAS already held exposure information, chemicals identified as a concern or for which regulatory action had been taken overseas, and chemicals detected in international studies analysing chemicals present in babies' umbilical cord blood.

Stage Two of IMAP began in July 2016. We are continuing to assess chemicals on the Inventory, including chemicals identified as a concern for which action has been taken overseas and chemicals that can be rapidly identified and assessed by using Stage One information. We are also continuing to publish information for chemicals on the Inventory that pose a low risk to human health or the environment or both. This work provides efficiencies and enables us to identify higher risk chemicals requiring assessment.

The IMAP framework is a science and risk-based model designed to align the assessment effort with the human health and environmental impacts of chemicals. It has three tiers of assessment, with the assessment effort increasing with each tier. The Tier I assessment is a high throughput approach using tabulated electronic data. The Tier II assessment is an evaluation of risk on a substance-by-substance or chemical category-by-category basis. Tier III assessments are conducted to address specific concerns that could not be resolved during the Tier II assessment.

These assessments are carried out by staff employed by the Australian Government Department of Health and the Australian Government Department of the Environment and Energy. The human health and environment risk assessments are conducted and published separately, using information available at the time, and may be undertaken at different tiers.

This chemical or group of chemicals are being assessed at Tier II because the Tier I assessment indicated that it needed further investigation.

For more detail on this program please visit:**www.nicnas.gov.au**

ACRONYMS & ABBREVIATIONS

Grouping Rationale

The chemicals in this group are closely related 6:2 fluorotelomer sulfonamide derivatives. In both cases, the sulfonamide is substituted with a 3-propyl amine group, which is further quaternised. In one chemical (6:2 fluorotelomer sulphonamide alkyl betaine (FTSAB); CAS No. 34455-29-3) the counterion is internal to the chemical (inner salt). The other chemical (6:2 fluorotelomer sulfonamide alkyl quaternary ammonium salt (FTSAQ); CAS No 94088-80-9) is a simple quaternary ammonium cation salt. The numbering in fluorotelomers refers to the number of fluorocarbons and hydrocarbons and in case of 6:2, it indicates six fluorinated carbons and two methylene carbons in the fluoroalkyl chain (Buck et al., 2011; Seow, 2013).

This group assessment also includes a chemical product that has been allocated its own CAS No. (listed on AICS). The product contains one of the fluorinated surfactants as an ingredient. The conclusions that apply to the fluorosurfactant ingredient will also apply to the chemical product.

The National Industrial Chemicals Notification and Assessment Scheme (NICNAS) has developed an action plan to assess and manage chemicals with a perfluorinated chain of four or more carbons which may degrade to perfluorinated carboxylic acids, perfluoroalkyl sulfonates and similar chemicals. This can be found on the NICNAS website under 'Data requirements for notification of new chemicals containing a perfluorinated carbon chain' (NICNASa).

The chemicals in this group are expected to biodegrade slowly in the environment and ultimately form short-chain PFCAs as the terminal degradants (NICNASd). Human health assessments for simple, short-chain PFCAs and their salts (direct precursors) have been published earlier using the toxicity data available for PFHxA and perfluorobutanoic acid (PFBA), in order to compare their toxicity profile with that of perfluorooctanoic acid (PFOA) (NICNASb).

Risks from direct exposure to the chemicals and secondary exposure to degradation products have been considered.

Import, Manufacture and Use

Australian

The 6:2 FTSAB (CAS No. 34455-29-3) has reported use as a surfactant in fire suppressant products.

Forafac 1157 identified by CAS No. 65256-46-4 was previously introduced to Australia, but has now been discontinued. This product contained CAS No. 34455-29-3 as an active ingredient.

No specific Australian use, import, or manufacturing information was identified for the 6:2 FTSAQ in this group (CAS No. 94088-80-9). Information collected by NICNAS in 2006 indicated PFHxA, PFPeA and their derivatives are not expected to be imported or manufactured in Australia.

It is noted that the chemicals in this group may be present in the environment due to release from pre-treated articles. However, release from this use is beyond the scope of this assessment.

International

The 6:2 FTSAB (CAS No. 34455-29-3) has reported use in fire-fighting foams and professional floor waxes and cleaners (REACH; SFT, 2007; Buck, et al., 2011; NICNASd; Place & Field, 2012). The chemical also has reported uses in inks and toners, paper chemicals and dyes, polymers, semiconductors and textile treatment products and dyes (REACH) and is used as an intermediate (Galleria Chemica).

Chemicals structurally related to 6:2 FSTAQ (CAS No. 94088-80-9) have been detected in fire-fighting foams and commercial surfactant concentrates (D'Agostino and Mabury, 2014; Place & Field, 2012).

Restrictions

Australian

The National Chemicals Working Group, Heads of EPAs Australia and New Zealand (HEPA) has developed the PFAS National Environmental Management Plan (PFAS NEMP) which provides governments with a risk-based framework for the environmental regulation of PFAS-contaminated materials and sites (HEPA, 2018).

Some state governments in Australia have introduced regulations regarding the management of PFAS-containing firefighting foams, which could impact the use, release, and disposal of chemicals in this group in these states. In South Australia, the Environmental Protection Agency prohibited potentially hazardous fluorinated firefighting foams on 30 January 2018 (EPA South Australia, 2018). This prohibition covers any firefighting foam containing a fluorinated organic compound or compounds, which would include the chemicals in this group.

The former Queensland Government Department of Environment and Heritage Protection (now the Department of the Environment and Science) has introduced a policy for the environmental management of firefighting foams (Queensland Government, 2016). In Queensland, foams containing short-chain fluorotelomers (i.e., fluorotelomers with a perfluorohexyl (C6) or shorter perfluoroalky chain) can be used in situations when they are the only viable option, after firefighting effectiveness, short and long-term health, safety and environmental risks and property protection characteristics have all been appropriately considered. However, end-users must be aware of the foam composition and it must be 'C6 purity compliant'. For the purposes of this policy, C6 purity compliant means it must not have greater than 50 mg/kg of total impurities in the concentrate for any compounds where the perfluorinated part of the carbon chain is longer than 6 carbon atoms (e.g. PFOA and PFOA precursors), but excluding PFOS which has a separate impurity limit of 10 mg/kg. In addition, there must be no releases to the environment and all releases must be fully contained on site, and all wastes must be disposed of as regulated waste to a facility authorised to accept such wastes (Queensland Government, 2016).

International

No known restrictions have been identified.

Existing Worker Health and Safety Controls

Hazard Classification

The chemicals are not listed on the Hazardous Substances Information System (HCIS) (Safe Work Australia).

Exposure Standards

Australian

No specific exposure standards are available for the chemicals.

International

No specific exposure standards are available for the chemicals.

Health Hazard Information

Health hazard data are only available for the 6:2 FTSAB. The final degradation products of the chemicals in this group are indicated to mainly be short-chain PFCAs including PFHxA; therefore, the human health hazard assessment of these chemicals is based on the toxicity profile of short-chain PFCAs. The toxicological profile for short-chain PFCAs (C4–C6) suggests potentially better human health outcomes and less bioaccumulation than long-chain perfluoroalkyl substances. There is no evidence of significant hepatotoxicity or carcinogenicity in repeated dose toxicity studies and developmental effects in mice occur at much higher doses in the short-chain PFCAs (NICNASb).

When PFCAs and their indirect precursors were analysed in maternal and cord blood serum, 6:2 FTSA was found to be the major component detected (Yang et al., 2016). However, based on data on the environmental biodegradation, the chemicals in this group are not likely to be a major source of 6:2 fluorotelomer sulfonic acid (6:2 FTSA; CAS No. 27619-97-2) (NICNASd); therefore, the toxicity of this chemical has not been considered as part of this assessment.

Acute Toxicity

Oral

Based on the reported median lethal doses (LD50) in experimental animals, the 6:2 FTSAB has low acute oral toxicity. The LD50 value from an Organisation for Economic Co-operation and Development (OECD) Test Guideline (TG) 425 study is >5000 mg/kg bw in rats. No mortality occurred and no other signs of toxicity were apparent during the study (REACH).

Dermal

Based on the reported LD50 value in experimental animals, the 6:2 FTSAB has low acute dermal toxicity. The LD50 value from an OECD TG 402 was >5000 mg/kg bw in rats. No mortality occurred and no other signs of toxicity were apparent during the study (REACH).

Inhalation

No data are available.

Corrosion / Irritation

Skin Irritation

The 6:2 FTSAB is not irritating to skin based on animal data.

In a skin irritation study following OECD TG 404, New Zealand White (NZW) rabbits (n = 3) were exposed to the chemical (85 % test substance in 15 % distilled water w/w) under a semiocclusive patch for 4 hours. No irritation was reported. The scores for erythema and oedema were 0 at all time-points (24, 48 and 72 hours) (REACH).

Eye Irritation

The 6:2 FTSAB is not irritating to eyes based on animal data.

In an OECD TG 405 eye irritation study, no corneal opacity, iritis, or conjunctival chemosis were observed. Conjunctival redness (score of 1) was noted in the treated eye of one rabbit and conjunctival discharge (score of 1) was noted was noted in the treated eye of all rabbits. Conjunctival irritation cleared in all rabbits within 24 hours (REACH).

Sensitisation

Skin Sensitisation

The 6:2 FTSAB is not expected to be a skin sensitiser based on animal data.

In a maximisation test (adjuvant test method) following OECD TG 406, the chemical was not sensitising when tested in Dunkin-Hartley guinea pigs (n = 10). For induction, the chemical was tested at 1 % and 5 % via intradermal route and epicutaneous routes, respectively. For challenge, the animals were topically exposed to the chemical at 1 %. No dermal reactions were observed in the study (REACH).

Repeated Dose Toxicity

Oral

Based on the available data, the 6:2 FTSAB is not expected to be harmful following repeated oral exposure.

In a 28-day oral toxicity study following OECD TG 407, the 6:2 FTSAB was administered to Sprague Dawley (SD) rats (6–12/sex/dose) by gavage at doses of 10, 40, 200 or 1000 mg/kg bw followed by a 2 week recovery period. All animals survived the study. Body weights were not affected apart from males receiving the highest dose; these had slightly reduced body weight and the end of the study. Soft stools were observed in animals receiving =200 mg/kg bw; however, this was reversible during the recovery period. No changes attributable to the chemical were observed in regards to haematology, clinical chemistry, urinalysis, and gross pathology. Centriloblular hepatic cell hypertrophy was observed in 3/6 males and single cell necrosis in 4/6 males at 1000 mg/kg bw/day at the end of the treatment period. Females had increased relative liver weights at the same dose. The liver effects were reversible during the recovery period. The reported no observed adverse effect level (NOAEL) from the study was 200 mg/kg bw/day based on liver effects at 1000 mg/kg bw/day (REACH).

Genotoxicity

Based on the available in vitro studies, the 6:2 FTSAB is not expected to be genotoxic.

The 6:2 FTSAB was negative in the following in vitro studies (REACH):

- a bacterial gene mutation assay following OECD TG 471 in *Salmonella typhimurium* strains TA1535, TA1537, TA98, TA100 and *Escherichia coli* WP2 exposed to concentrations up to 5000 µg/plate with metabolic activation and up to 1250 µg/plate without metabolic activation;
- a mammalian cell gene mutation study following OECD TG 476 in mouse lymphoma cells exposed to concentrations up to 500 µg/mL with without metabolic activation for 4 hours and concentrations up to 93.8 µg/mL for 24 hours without metabolic activation; and
- a chromosome aberration study in mammalian cells following OECD TG 473 in Chinese hamster lung cells at concentrations up to 5000 µg/mL for 6 hours or up to 78.1 µg/mL for 24 hours with and without metabolic activation.

Carcinogenicity

No data are available.

Reproductive and Developmental Toxicity

No data on effects on fertility are available. Based on the available information, the 6:2 FTSAB is not expected to be toxic to foetal development.

In a prenatal developmental toxicity study following OECD TG 414, the 6:2 FTSAB was administered by gavage at doses of 0, 25, 150, or 1000 mg/kg bw/day to pregnant SD rats (22/dose) during gestation days (GD) 6–15. All animals survived the study. Clinical signs of maternal toxicity included reduced body weight gain and reduced food consumption at the highest dose (1000 mg/kg bw/day). The mean number of implantation sites, resorptions, live foetuses, mean sex ratio and foetal weights were comparable across all groups. There were no chemical-related foetal external, visceral, or skeletal malformations or variations observed at any dose level. The reported NOAEL for maternal toxicity was 150 mg/kg bw/day, based on reduced maternal body weight gain at 1000 mg/kg bw/day. The NOAEL for developmental toxicity was 1000 mg/kg bw/day (REACH).

In a 28-day repeated dose toxicity study (see **Repeated dose toxicity: Oral**), increased relative weights of testes was found in high-dose males (1000 mg/kg bw/day) at the end of the 2-week recovery period. No other reproductive organ effects were reported (REACH).

Risk Characterisation

Critical Health Effects

Based on the available data, no critical health effects relating to direct exposure to the chemicals have been identified.

The chemicals in this group have the potential to degrade to short-chain perfluorocarboxylic acids (PFCAs) containing 4–5 perfluorinated carbons. The data available indicate that the toxicological profile for short-chain PFCAs (C4–C6) gives rise to potentially better human health outcomes and the chemicals have lower bioaccumulation potential than long-chain perfluoroalkyl substances (NICNASb). Chronic low-level effects on human health, such as hepatotoxicity and carcinogenicity, have not been identified.

Public Risk Characterisation

Based on the available use information, the chemicals in this group unlikely to be widely available for consumer uses. Hence, the public risk from direct use of these chemicals is not considered to be unreasonable.

Secondary exposure to short-chain PFCAs in the environment

Public exposure to short-chain PFCAs could occur through secondary exposure in the environment. It is noted that the perfluorinated carboxylic acid degradants formed from the parent chemicals in this group may have multiple sources. These perfluorinated components are highly persistent and environmental levels can continue to increase over time due to indirect release pathways (NICNASc).

The available data indicate that short-chain PFCAs have lower toxicity and are more rapidly eliminated than the long-chain perfluoroalkyl substances. Chronic low-level effects on human health have not been identified. The chemicals in the short-chain PFCA group are persistent in the environment, but have a short half-life in humans. Further assessment of the chemicals in this group may be necessary if information becomes available indicating adverse health effects from either the parent chemicals or their principal degradation products.

Occupational Risk Characterisation

Based on the available use information, the chemicals or their products are not manufactured in Australia. The chemicals are not likely to be used in significant quantities in Australia. Further assessment of the chemicals in this group may be necessary to inform the risk to workers if information becomes available indicating that these chemicals are introduced into Australia in significant quantities.

Long-term occupational exposure to very low concentrations of these chemicals and the degradation products could occur while using formulated products.

NICNAS Recommendation

The chemicals in this group have been assessed as having the potential to give rise to short-chain perfluorocarboxylic acids (PFCAs). Limited available toxicological data on these chemicals indicate a lower toxicity profile compared with long-chain PFCAs. However, should information become available indicating adverse health effects, further assessment of the chemicals in this group may be necessary to assess the risk of secondary exposure to short-chain PFCAs.

Introducers and users of the chemicals in this group should be aware of and comply with the federal, state and territory regulations and policies and industry recommendations regarding their use in AFFFs. Adherence to these regulations and practices where relevant will minimise the risks to humans from secondary exposure via the environment from the use of these chemicals in AFFFs.

Introducers of the chemicals should specify the quantity of long-chain PFAS impurities present in firefighting foam formulations to environmental regulators and end-users to ensure that effective best management practices are implemented prior to an emergency and during their use.

It is noted that the IMAP Human Health Tier II Assessment for Short-Chain Perfluorocarboxylic Acids (PFCAs) and their Direct Precursors (NICNASb) found that sufficient information was available to demonstrate that short-chain perfluorocarboxylic acids have a lower toxicity profile compared to PFOA, and it was recommended that the assessment be included in the action plan contained in Appendix G of the Handbook for Notifiers (NICNASa). This should be considered during the application of the action plan to any chemicals which may degrade to short-chain perfluorocarboxylic acids.

Regulatory Control

Advice for industry

Control measures to minimise the exposure to the chemicals should be implemented in accordance with the hierarchy of controls. Approaches to minimise the exposure include substitution, isolation and engineering controls. Measures required to eliminate or minimise exposure arising from storing, handling and using a hazardous chemical depend on the physical form and the manner in which the chemicals are used. Examples of control measures that could minimise the risk include, but are not limited to:

- minimising manual processes and work tasks through automating processes;
- work procedures that minimise splashes and spills;
- regularly cleaning equipment and work areas; and
- using protective equipment that is designed, constructed, and operated to ensure that the worker does not come into contact with the chemicals.

Guidance on managing risks from hazardous chemicals are provided in the Managing risks of hazardous chemicals in the workplace—Code of practice available on the Safe Work Australia website.

Personal protective equipment should not solely be relied upon to control risk and should only be used when all other reasonably practicable control measures do not eliminate or sufficiently minimise risk. Guidance in selecting personal protective equipment can be obtained from Australian, Australian/New Zealand or other approved standards.

Obligations under workplace health and safety legislation

Information in this report should be taken into account to help meet obligations under workplace health and safety legislation as adopted by the relevant state or territory. This includes, but is not limited to:

- ensuring that hazardous chemicals are correctly classified and labelled;
- ensuring that (material) safety data sheets ((M)SDS) containing accurate information about the hazards (relating to both health hazards and physicochemical (physical) hazards) of the chemicals are prepared; and
- managing risks arising from storing, handling and using a hazardous chemical.

Your work health and safety regulator should be contacted for information on the work health and safety laws in your jurisdiction.

Information on how to prepare an (M)SDS and how to label containers of hazardous chemicals are provided in relevant codes of practice such as the Preparation of safety data sheets for hazardous chemicals—Code of practice and Labelling of workplace hazardous chemicals—Code of practice, respectively. These codes of practice are available from the Safe Work Australia website.

A review of the physical hazards of these chemicals has not been undertaken as part of this assessment.

References

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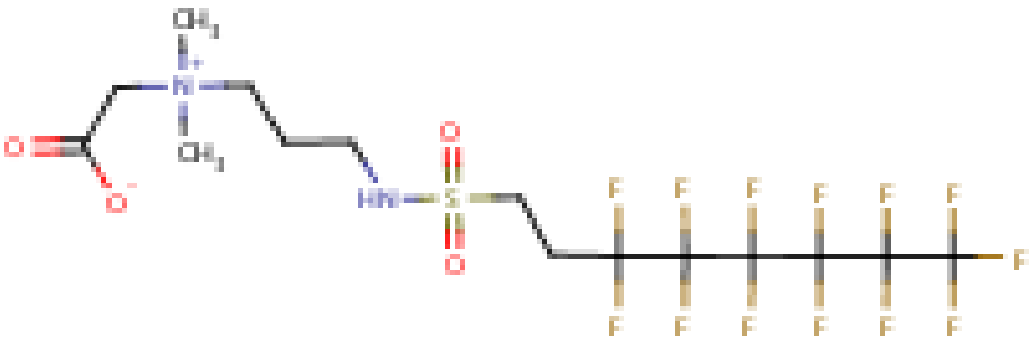
Last Update 12 December 2019

Chemical Identities

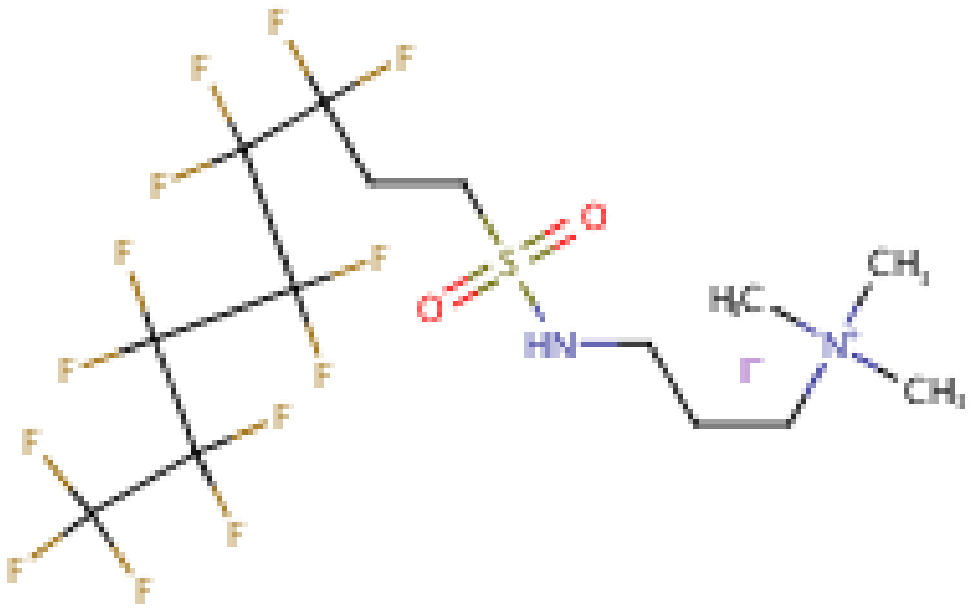
Chemical Name in the Inventory and Synonyms	**1-Propanaminium, N-(carboxymethyl)-N,N-dimethyl-3-[[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulfonyl]amino]-, hydroxide, inner salt** 1-propanaminium, N-(carboxymethyl)-N,N-dimethyl-3-[(1,1,2,2-tetrahydroperfluorooctyl)sulfonylamino N-(carboxymethyl)-N,N-dimethyl-3-[[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulfonyl]amino]-1-propanaminium, inner salt 6:2 fluorotelomer sulfonamide alkyl betaine (6:2 FTSAB) polyfluoroalkyl betaine
CAS Number	34455-29-3
Structural Formula	



Molecular Formula	C15H19F13N2O4S
Molecular Weight	570.4

Chemical Name in the Inventory and Synonyms	**Forafac 1157** Perfluoroalkyl betaine
CAS Number	65256-46-4
Structural Formula	**No Structural Diagram Available**

Molecular Formula	Unspecified
Molecular Weight	

Chemical Name in the Inventory and Synonyms	**1-Propanaminium, N,N,N-trimethyl-3-[[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulfonyl]amino]-, iodide** trimethyl-3-(((3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulphonyl)amino)propylammonium iodide 6:2 fluorotelomer sulfonamide propyltrimethylammonium iodide (6:2 FTSAQ)
CAS Number	94088-80-9
Structural Formula	
Molecular Formula	C14H20F13N2O2S.I
Molecular Weight	654.264

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