Indirect precursors to perfluorooctanesulfonate (PFOS): Environment tier II assessment

8 March 2019

CAS Registry Numbers: 31506-32-8, 1691-99-2, 24448-09-7, 40630-61-3, 376-14-7, 423-82-5, 127133-66-8, 594864-11-6, 68298-62-4, 68329-56-6, 68555-90-8, 68555-91-9, 68555-92-0, 68568-77-4, 68797-76-2, 68867-60-7, 68909-15-9, 70776-36-2, 92265-81-1, 68227-96-3, 68298-78-2, 68299-39-8, 68586-14-1, 68867-62-9, 70900-40-2, 68081-83-4, 94313-84-5, 2991-51-7, 161074-58-4, 185630-90-4, 253682-96-1, 91081-99-1, 192662-29-6, 68649-26-3, 68608-14-0, 68608-13-9, 306973-47-7, 306975-56-4, 3820-83-5, 2250-98-8, 30381-98-7, 67969-69-1, 29117-08-6, 37338-48-0, 68958-61-2, 1652-63-7, 38006-74-5, 67939-88-2, 68298-11-3, 94133-90-1, 57589-85-2, 68891-96-3, 75260-69-4, 94133-91-2, 944578-05-6

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.

Disclaimer

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Acronyms & Abbreviations

Grouping Rationale

This Tier II assessment considers the environmental risks associated with the industrial uses of a group of 55 chemicals. The chemicals in this group are structurally related compounds in that they all contain a chain of eight perfluorinated carbons linked to a terminal sulfonamide or sulfonic ester group.

NICNAS has developed an action plan to assess and manage chemicals which may degrade to perfluorinated carboxylic acids, perfluoroalkyl sulfonates and similar chemicals (NICNAS, 2018a). The primary assumption outlined in this action plan is that chemicals with a perfluorinated chain terminated by a sulfonyl group will degrade to the perfluoroalkyl sulfonate. On this basis the chemicals in this group are each considered to have the potential to degrade into the environmentally hazardous perfluorooctanesulfonate anion (PFOS).

Perfluorooctanesulfonic acid, perfluorooctanesulfonates, perfluorooctanesulfonamides and perfluorooctanesulfonyls are listed on Annex III of the *Rotterdam Convention on the Prior Informed Consent Procedure for Certain Hazardous Chemicals and*

*Pesticides in International Trade (*the Rotterdam Convention). In addition, perfluorooctanesulfonic acid and certain PFOS-related substances have recently been identified as Persistent Organic Pollutants (POPs) under Annex B of the *Stockholm Convention on Persistent Organic Pollutants* (the Stockholm Convention). Further information on PFOS can be found in the Environment Tier II Assessment of the Direct Precursors to Perfluorooctanesulfonate (PFOS) group (NICNAS, 2015a).

The degradation of PFOS is very slow compared with its rate of formation from degradation of the precursors and PFOS will be the final degradant from multiple precursors. Therefore, the amount of PFOS in the environment (general or local) is expected to be higher than that of any of the precursors. It will therefore be assumed for the purposes of this assessment that the primary risk posed by the chemicals in this group results from the release of PFOS to the environment. The IMAP-Environment Tier II assessment for Direct Precursors to Perfluorooctanesulfonate (PFOS) (NICNAS, 2015a) has been used as a reference assessment.

Chemical Identity

In this assessment, "PFOS" is used to denote the conjugate base anion of perfluorooctanesulfonic acid (i.e. the perfluorooctanesulfonate anion). However, it is noted that this descriptor is commonly used in relation to a range of substances which may easily form the anion in water, such as the parent acid and salts of the acid.

Acronyms for certain chemicals in this group have been taken from a list of recommended acronyms and other terminology recently compiled to facilitate clear and unambiguous communication regarding the major classes of industrially important perfluoroalkyl and polyfluoroalkyl substances (Buck, et al., 2011).

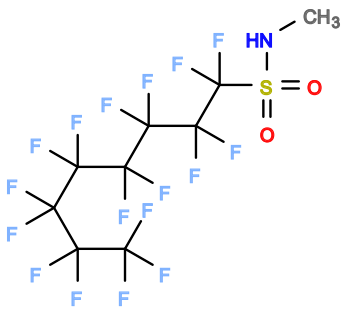
This assessment includes a range of neutral and ionic organic chemicals, polymers, telomers, and chemicals that are in the category of unknown or variable composition, complex reaction products or biological materials (UVCBs). The chemicals in this assessment have been sub-grouped based on similar structural properties below for presentation purposes.

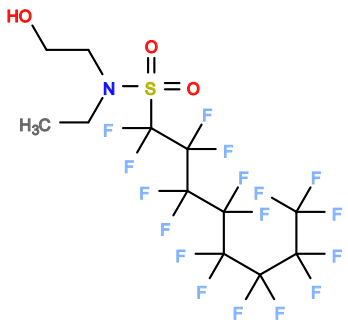
Structural information is presented where it is available. For polymers and telomers, constituent monomers are presented. Due to the typically variable size and structure of polymer molecules, the molecular formula and molecular weight for these substances are not presented.

Where insufficient structural information is available, the CAS RN and chemical name are presented only.

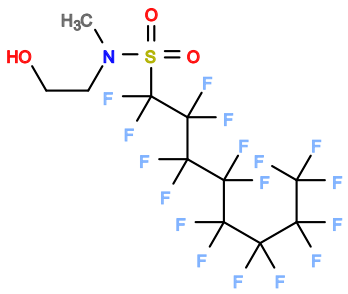
Neutral Organic Derivatives of Perfluorooctanesulfonamides

CAS RN	31506-32-8
Chemical Name	1-Octanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-*N*-methyl-
Synonyms	MeFOSA *N*-methylperfluorooctanesulfonamide
Structural Formula	

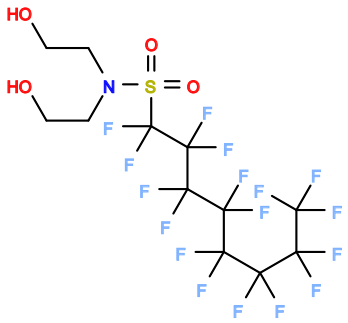
	
Molecular Formula	$C_9H_4F_{17}NO_2S$
Molecular Weight (g/mol)	513.17
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)NC

CAS RN	1691-99-2
Chemical Name	1-Octanesulfonamide, *N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-*N*-(2-hydroxyethyl)-
Synonyms	EtFOSE *N*-ethylperfluorooctanesulfonamidoethanol
Structural Formula	
Molecular Formula	$C_{12}H_{10}F_{17}NO_3S$

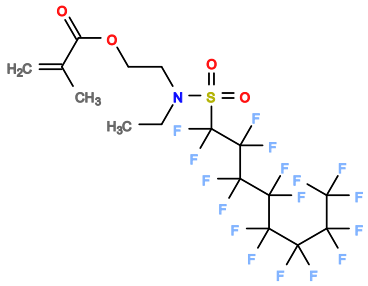
Molecular Weight (g/mol)	571.25
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCO)CC

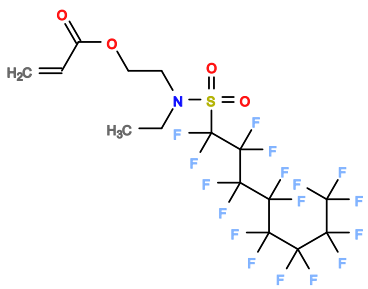
CAS RN	24448-09-7
Chemical Name	1-Octanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-*N*-(2-hydroxyethyl)-*N*-methyl-
Synonyms	MeFOSE *N*-methylperfluorooctanesulfonamidoethanol
Structural Formula	
Molecular Formula	$C_{11}H_8F_{17}NO_3S$
Molecular Weight (g/mol)	557.22
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(C)CCO

CAS RN	40630-61-3

Chemical Name	1-Octanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-*N*,*N*-bis(2-hydroxyethyl)-
Synonyms	*N*,*N*-bis(2-hydroxyethyl)perfluorooctanesulfonamide
Structural Formula	
Molecular Formula	$C_{12}H_{10}F_{17}NO_4S$
Molecular Weight (g/mol)	587.25
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)N(CCO)CCO

CAS RN	376-14-7
Chemical Name	2-Propenoic acid, 2-methyl-, 2-[ethyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl ester
Synonyms	EtFOSMAC *N*-ethylperfluorooctanesulfonamidoethyl methacrylate
Structural Formula	

	
Molecular Formula	$C_{16}H_{14}F_{17}NO_4S$
Molecular Weight (g/mol)	639.32
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOC(=O)C(=C)C)CC

CAS RN	423-82-5
Chemical Name	Acrylic acid, ester with *N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-*N*-(2-hydroxyethyl)-1-octanesulfonamide
Synonyms	EtFOSAC *N*-ethylperfluorooctanesulfonamidoethyl acrylate
Structural Formula	
Molecular Formula	$C_{15}H_{12}F_{17}NO_4S$
Molecular Weight	625.30

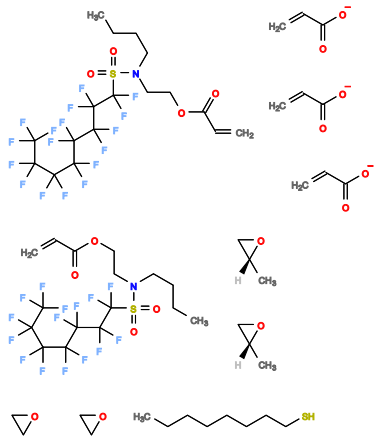
(g/mol)	
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOC(=O)C=C)CC

Methacrylate and Acrylate Polymers with Perfluorooctanesulfonamide Side Chains

CAS RN	127133-66-8
Chemical Name	2-Propenoic acid, 2-methyl-, polymers with butyl methacrylate, lauryl methacrylate and 2-[methyl[(perfluoro-C4-8-alkyl)sulfonyl]amino]ethyl methacrylate

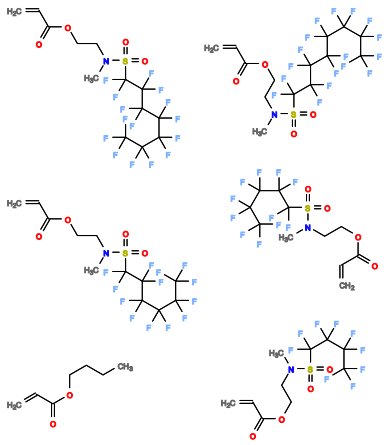
CAS RN	594864-11-6
Chemical Name	2-Propenoic acid, butyl ester, polymer with 2-[butyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl 2-propenoate and 2-methylpropyl 2-propenoate

CAS RN	68298-62-4
Chemical Name	2-Propenoic acid, 2-[butyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl ester, telomer with 2-[butyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, methyloxirane polymer with oxirane di-2-propenoate, methyloxirane polymer with oxirane mono-2-propenoate and 1-octanethiol
Synonyms	*N*-butylperfluorooctanesulfonamidoethyl acrylate telomer with *N*-butylperfluorooctanesulfonamidoethyl acrylate propylene glycol polymer with ethylene glycol-propylene glycol copolymer diacrylate with ethylene glycol-propylene glycol copolymer monoacrylate and n-octyl mercaptan
Structural Formula	

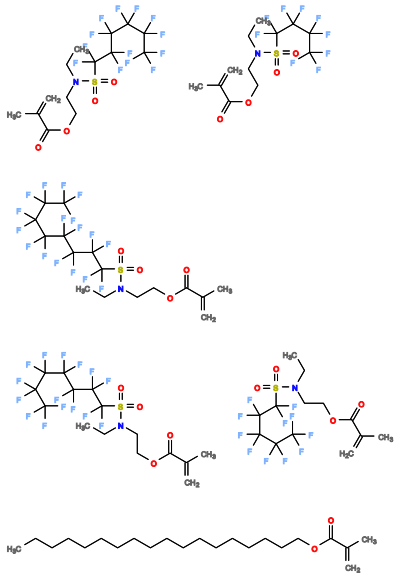
	
SMILES	C(C=C)(=O)OCC[N@@](S(C(F)(F)C(C(C(C(C(C(C F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(=O)=O)CCCC. C(C=C)(=O)[O-].C(S)CCCCCCC.O1CC1.O1[C@@H] (C1)C.C(C=C)(=O)[O-].C(C=C)(=O)[O-].O1CC1.O1 [C@@H](C1)C.C(C=C)(=O)OCC[N@@](S(=O)(=O) C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F) CCCC

CAS RN	68329-56-6
Chemical Name	2-Propenoic acid, eicosyl ester, polymer with 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl 2-propenoate, hexadecyl 2-propenoate, 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-propenoate and octadecyl 2-propenoate

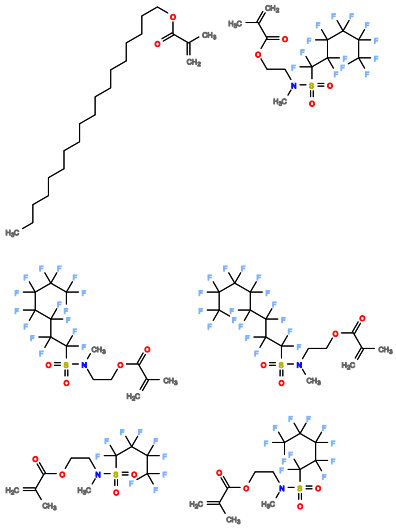
CAS RN	68555-90-8
Chemical Name	2-Propenoic acid, butyl ester, polymer with 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl 2-propenoate, 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-propenoate and 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl2-propenoate
Synonyms	butyl acrylate, polymer with *N*-methylperfluoroalkyl-C4-8-sulfonamidoethyl

	acrylates
Structural Formula	
SMILES	C(C=C)(=O)OCC[N@@](S(=O)(=O)C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)C.C(C=C)(=O)OCC[N@@](S(C(F)(F)C(F)(F)C(F)(F)C(C(C(F)(F)F)(F)F)(F)F)(=O)=O)C.C(C=C)(=O)OCC[N@@](S(C(C(C(C(C(C(F)(C(F)(F)F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(=O)=O)C.C(C=C)(=O)OCC[N@@](S(=O)(=O)C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)C.C(C=C)(=O)OCC[N@@](C)S(=O)(=O)C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F.C(C=C)(=O)OCCCC

CAS RN	68555-91-9
Chemical Name	2-Propenoic acid, 2-methyl-, 2-[ethyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl ester, polymer with 2-[ethyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate and octadecyl 2-methyl-2-propenoate
Synonyms	*N*-ethylperfluorooctanesulfonamidoethyl methacrylate, polymer with *N*-ethylperfluorooalkyl-C4-7-sulfonamidoethyl methacrylates and stearyl methacrylate
Structural Formula	

	
SMILES	C(C(=C)C)(=O)OCCCCCCCCCCCCCCCCCC. C(C(=C)C)(=O)OCC[N@@](S(C(C(C(C(F)(C (F)(F)F)F)(F)F)(F)F)(F)F)(F)F)(=O)=O)CC.C(C(=C)C) (=O)OCC[N@@](S(=O)(=O)C(C(C(C(C(C(F)(F)F) (F)F)(F)F)(F)F)(F)F)(F)F)(F)F)CC.C(C(=C)C)(=O)OCC [N@@](S(=O)(=O)C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F) (F)F)(F)F)(F)F)(F)F)CC.C(C(=C)C)(=O)OCC[N@@] (S(=O)(=O)C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)CC. C(C(=C)C)(=O)OCC[N@@](S(=O)(=O)C(C(C(C(C(C(C(C (F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)CC

CAS RN	68555-92-0
Chemical Name	2-Propenoic acid, 2-methyl-, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl ester, polymer with 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate and octadecyl 2-methyl-2-propenoate
Synonyms	*N*-methylperfluorooctanesulfonamidoethyl methacrylate, polymer with *N*-methylperfluorooalkyl-C4-7-sulfonamidoethyl methacrylates and stearyl methacrylate
Structural Formula	

	
SMILES	CC(C(=O)OCC[N@@](C)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)=C.CC(C(=O)OCC[N@@](C)S(=O)(=O)C(C(C(C(C(C(F)(F)C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)=C.CC(C(OCC[N@@](C)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(C(C(F)(F)F)(F)F)(F)F)(F)F)=O)=C.CC(C(OCC[N@@](C)S(=O)(=O)C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)=O)=C.CC(C(OCC[N@@](C)S(=O)(=O)C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)=O)=C.CC(C(OCCCCCCCCCCCCCCCCCCCC)=O)=C

CAS RN	68568-77-4
Chemical Name	2-Propenoic acid, 2-methyl-, 2-[ethyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl ester, polymer with 2-chloro-1,3-butadiene, 2-[ethyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate and 2-[ethyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate

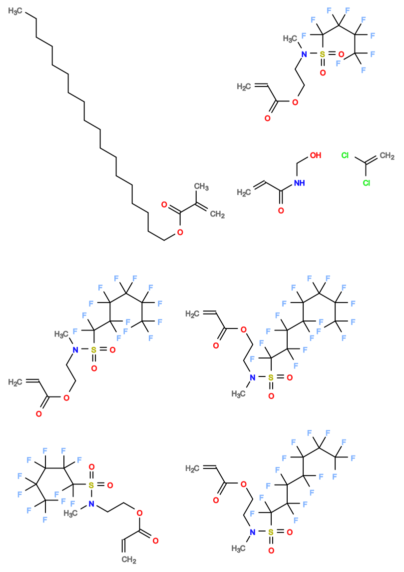
CAS RN	68797-76-2
Chemical Name	2-Propenoic acid, 2-methyl-, 2-ethylhexyl ester, polymer with 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl 2-propenoate, 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-propenoate, 2-

	[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-propenoate and oxiranylmethyl 2-methyl-2-propenoate

CAS RN	68867-60-7
Chemical Name	2-Propenoic acid, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl ester, polymer with 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-propenoate and .alpha.-(1-oxo-2-propenyl)-.omega.-methoxypoly(oxy-1,2-ethanediyl)

CAS RN	68909-15-9
Chemical Name	2-Propenoic acid, eicosyl ester, polymer with branched octyl 2-propenoate, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl 2-propenoate, 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-propenoate, octadecyl 2-propenoate and .alpha.-(1-oxo-2-propenyl)-.omega.-methoxypoly(oxy-1,2-ethanediyl)

CAS RN	70776-36-2
Chemical Name	2-Propenoic acid, 2-methyl-, octadecyl ester, polymer with 1,1-dichloroethene, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl 2-propenoate, *N*-(hydroxymethyl)-2-propenamide, 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl2-propenoate and 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-propenoate
Synonyms	stearyl methacrylate, polymer with 1,1-dichloroethene, n-methylolacrylamide and *N*-methylperfluoro-C4-8-sulfonamidoethyl acrylates

Structural Formula	
SMILES	C(C=C)(=O)OCC[N@@](S(=O)(=O)C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)C.C(C=C)(=O)OCC[N@@](S(=O)(=O)C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)C.C(C=C)(=O)OCC[N@@](S(=O)(=O)C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)C.C(C=C)(=O)NCO.C(C=C)(=O)OCC[N@@](C)S(=O)(=O)C(C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F.C(=C)(Cl)Cl.C(OCCCCCCCCCCCCCCCCCC)(C(=C)C)=O.C(C=C)(=O)OCC[N@@](C)S(=O)(=O)C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F

CAS RN	92265-81-1
Chemical Name	Ethanaminium, *N*,*N*,*N*-trimethyl-2-[(2-methyl-1-oxo-2-propenyl)oxy]-, chloride, polymer with 2-ethoxyethyl 2-propenoate, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl 2-propenoate and oxiranylmethyl 2-methyl-2-propenoate

Methacrylate and Acrylate Telomers with Perfluorooctanesulfonamide Side Chains

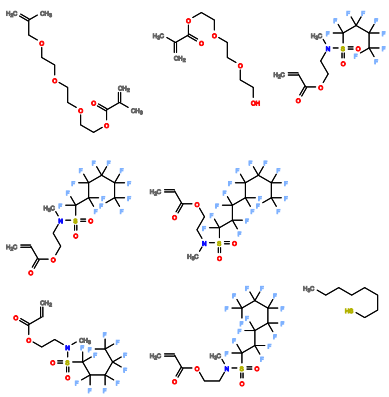
CAS RN	68227-96-3
Chemical Name	2-Propenoic acid, butyl ester, telomer with 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl 2-propenoate, 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, .alpha.-(2-

	methyl-1-oxo-2-propenyl)-.omega.-hydroxypoly(oxy-1,4-butanediyl), .alpha.-(2-methyl-1-oxo-2-propenyl)-.omega.-[(2-methyl-1-oxo-2-propenyl)oxy]poly(oxy-1,4-butanediyl), 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate,2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-propenoate and 1-octanethiol

CAS RN	68298-78-2
Chemical Name	2-Propenoic acid, 2-methyl-, 2-[[[[5-[[[2-[ethyl[(heptadecafluorooctyl)sulfonyl]amino]ethoxy]carbonyl]amino]-2-methylphenyl]amino]carbonyl]oxy]propyl ester, telomer with butyl 2-propenoate, 2-[[[[5-[[[2-[ethyl[(nonafluorobutyl)sulfonyl]amino]ethoxy]carbonyl]amino]-2-methylphenyl]amino]carbonyl]oxy]propyl 2-methyl-2-propenoate, 2-[[[[5-[[[2-[ethyl[(pentadecafluoroheptyl)sulfonyl]amino]ethoxy]carbonyl]amino]-2-methylphenyl]amino]carbonyl]oxy]propyl 2-methyl-2-propenoate, 2-[[[[5-[[[2-[ethyl[(tridecafluorohexyl)sulfonyl]amino]ethoxy]carbonyl]amino]-2-methylphenyl]amino]carbonyl]oxy]propyl 2-methyl-2-propenoate, 2-[[[[5-[[[2-[ethyl[(undecafluoropentyl)sulfonyl]amino]ethoxy]carbonyl]amino]-2-methylphenyl]amino]carbonyl]oxy]propyl 2-methyl-2-propenoate, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl 2-propenoate, 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-propenoate and 1-octanethiol

CAS RN	68299-39-8
Chemical Name	2-Propenoic acid, 2-methyl-, 4-[[(heptadecafluorooctyl)sulfonyl]methylamino]butyl ester, telomer with butyl 2-propenoate, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl 2-propenoate, 4-[methyl[(nonafluorobutyl)sulfonyl]amino]butyl 2-methyl-2-propenoate, 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, .alpha.-(2-methyl-1-oxo-2-propenyl)-.omega.-hydroxypoly(oxy-1,4-butanediyl), .alpha.-(2-methyl-1-oxo-2-propenyl)-.omega.-[(2-methyl-1-oxo-2-propenyl)oxy]poly(oxy-1,4-butanediyl), 4-

	[methyl[(pentadecafluoroheptyl)sulfonyl]amino]butyl 2-methyl-2-propenoate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, 4-[methyl[(tridecafluorohexyl)sulfonyl]amino]butyl 2-methyl-2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-propenoate, 4-[methyl[(undecafluoropentyl)sulfonyl]amino]butyl 2-methyl-2-propenoate, 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-propenoate and 1-octanethiol

CAS RN	68586-14-1
Chemical Name	2-Propenoic acid, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl ester, telomer with 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, .alpha.-(2-methyl-1-oxo-2-propenyl)-.omega.-hydroxypoly(oxy-1,2-ethanediyl), .alpha.-(2-methyl-1-oxo-2-propenyl)-.omega.-[(2-methyl-1-oxo-2-propenyl)oxy]poly(oxy-1,2-ethanediyl), 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-propenoate and 1-octanethiol
Synonyms	*N*-methylperfluorooctanesulfonamidoethyl acrylate, telomer with poly(ethylene glycol) dimethacrylate, poly(ethylene glycol) monomethacrylate, *N*-methylperfluoroalkyl-C4-7-sulfonamidoethyl acrylate and n-octyl mercaptan
Structural Formula	
SMILES	O=C(OCCOCCOCCOCC(=C)C)C(C)=C. O=C(OCCOCCOCCO)C(C)=C.C(CCCCCCC)S. C(C=C)(=O)OCC[N@@](S(C(F)(C(F)(F)C(F)(F) C(F)(F)C(F)(F)F)F)(=O)=O)C.C(C=C)(=O)OCC [N@@](S(=O)(=O)C(C(C(C(C(C(F)(F)F)(F)F)(F)F) (F)F)(F)F)(F)F)C.C(C=C)(=O)OCC[N@@](S(=O) (=O)C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)

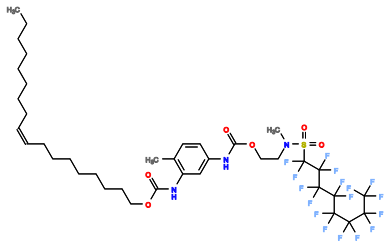
	(F)F)C.C(C=C)(=O)OCC[N@@](S(=O)(=O)C(C(C(C (F)(F)F)(F)F)(F)F)(F)F)C.C(C=C)(=O)OCC[N@@](C) S(=O)(=O)C(C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F) (F)F)(F)F)(F)F)(F)F

CAS RN	68867-62-9
Chemical Name	2-Propenoic acid, 2-methyl-, 2-[ethyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl ester, telomer with 2-[ethyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 1-octanethiol and .alpha.-(1-oxo-2-propenyl)-.omega.-methoxypoly(oxy-1,2-ethanediyl)

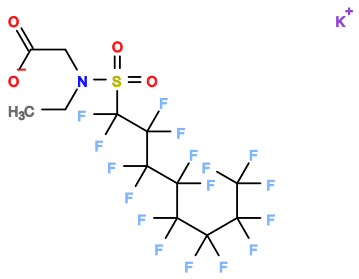
CAS RN	70900-40-2
Chemical Name	2-Propenoic acid, 2-methyl-, 2-[[[[5-[[[4-[[(heptadecafluorooctyl)sulfonyl]methylamino] butoxy]carbonyl]amino]-2-methylphenyl]amino] carbonyl]oxy]propyl ester, telomer with butyl 2-propenoate, 2-[[(heptadecafluorooctyl)sulfonyl] methylamino]ethyl 2-propenoate, 2-[[[[2-methyl-5-[[[4-[methyl[(nonafluorobutyl)sulfonyl]amino]butoxy] carbonyl]amino]phenyl]amino]carbonyl]oxy]propyl 2-methyl-2-propenoate, 2-[[[[2-methyl-5-[[[4-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]butoxy] carbonyl]amino]phenyl]amino]carbonyl]oxy]propyl 2-methyl-2-propenoate, 2-[[[[2-methyl-5-[[[4-[methyl[(tridecafluorohexyl)sulfonyl]amino]butoxy] carbonyl]amino]phenyl]amino]carbonyl]oxy]propyl 2-methyl-2-propenoate, 2-[[[[2-methyl-5-[[[4-[methyl[(undecafluoropentyl)sulfonyl]amino]butoxy] carbonyl]amino]phenyl]amino]carbonyl]oxy]propyl 2-methyl-2-propenoate, 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-propenoate and 1-octanethiol

Carbamate Esters of Perfluorooctanesulfonamides

CAS RN+	68081-83-4
Chemical Name	Carbamic acid, (4-methyl-1,3-phenylene)bis-, bis[2-[ethyl[(perfluoro-C4-8-alkyl)sulfonyl]amino]ethyl] ester

CAS RN	94313-84-5
Chemical Name	Carbamic acid, [5-[[[2-[[(heptadecafluorooctyl)sulfonyl]methylamino] ethoxy]carbonyl]amino]-2-methylphenyl]-, 9-octadecenyl ester, (*Z*)-
Synonyms	(*Z*)-octadec-9-enyl [5-[[[2-[[(perfluorooctyl)sulphonyl]methylamino] ethoxy]carbonyl]amino]-o-tolyl]carbamate
Structural Formula	
Molecular Formula	$C_{38}H_{50}F_{17}N_3O_6S$
Molecular Weight (g/mol)	999.86
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(C)CCOC(=O)Nc1cc(NC(=O)OCCCCCCCCC/C=C\CCCCCCCC)c(C)cc1

Carboxylic acid, Ester and Amide Derivatives of Perfluorooctanesulfonamides

CAS RN	2991-51-7
Chemical Name	Glycine, *N*-ethyl-*N*-[(heptadecafluorooctyl)sulfonyl]-, potassium salt
Synonyms	potassium EtFOSAA potassium *N*-ethylperfluorooctanesulfonamido acetate
Structural Formula	
Molecular Formula	$C_{12}H_7F_{17}KNO_4S$
Molecular Weight (g/mol)	623.32
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F) C(F)(F)C(F)(F)F)S(=O)(=O)N(CC(=O)[O-])CC.[K+]

CAS RN	75260-69-4
Chemical Name	Glycine, *N*-[(heptadecafluoroctyl)sulfonyl]-, monopotassium salt
Synonyms	potassium FOSAA

CAS RN	161074-58-4
Chemical Name	Fatty acids, C18-unsatd., trimers, reaction products with

	1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8 heptadecafluoro-*N*-(2-hydroxyethyl)-*N*-methyl-1-octanesulfonamide, 1,1,2,2,3,3,4,4,4-nonafluoro-*N*-(2-hydroxyethyl)-*N*-methyl-1-butanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-*N*-(2-hydroxyethyl)-*N*-methyl-1-heptanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-*N*-(2-hydroxyethyl)-*N*-methyl-1-hexanesulfonamide and 1,1,2,2,3,3,4,4,5,5,5-undecafluoro-*N*-(2-hydroxyethyl)-*N*-methyl-1-pentanesulfonamide

CAS RN	185630-90-4
Chemical Name	9-Octadecenoic acid (*Z*)-, reaction products with *N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-*N*-(2-hydroxyethyl)-1-octanesulfonamide

CAS RN	253682-96-1
Chemical Name	1-Octanesulfonamide, *N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-, reaction products with succinic anhydride monopolyisobutylene derivs.

CAS RN	91081-99-1
Chemical Name	Sulfonamides, C4-8-alkane, perfluoro, *N*-(hydroxyethyl)-*N*-methyl, reaction products with epichlorohydrin, adipates (esters)

CAS RN	192662-29-6
Chemical Name	Sulfonamides, C4-8-alkane, perfluoro, *N*-[3-(dimethylamino)propyl], reaction products with acrylic acid

Urethane Polymers Incorporating Perfluorooctanesulfonamides

CAS RN	68649-26-3

Chemical Name	1-Octanesulfonamide, *N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-*N*-(2-hydroxyethyl)-, reaction products with *N*-ethyl-1,1,2,2,3,3,4,4,4-nonafluoro-*N*-(2-hydroxyethyl)-1-butanesulfonamide, *N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-*N*-(2-hydroxyethyl)-1-heptanesulfonamide, *N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-*N*-(2-hydroxyethyl)-1-hexanesulfonamide, *N*-ethyl-1,1,2,2,3,3,4,4,5,5,5-undecafluoro-*N*-(2-hydroxyethyl)-1-pentanesulfonamide, polymethylenepolyphenylene isocyanate and stearyl alcohol

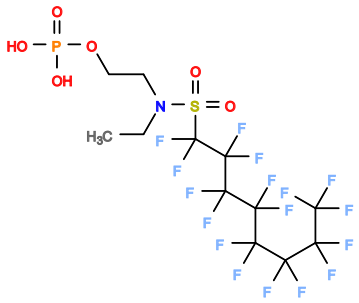
CAS RN	68608-14-0
Chemical Name	Sulfonamides, C4-8-alkane, perfluoro, *N*-ethyl-*N*-(hydroxyethyl), reaction products with 1,1'-methylenebis[4-isocyanatobenzene]

CAS RN	68608-13-9
Chemical Name	Sulfonamides, C4-8-alkane, perfluoro, *N*-ethyl-*N*-(hydroxyethyl), reaction products with 1,3-diisocyanatomethylbenzene polymer

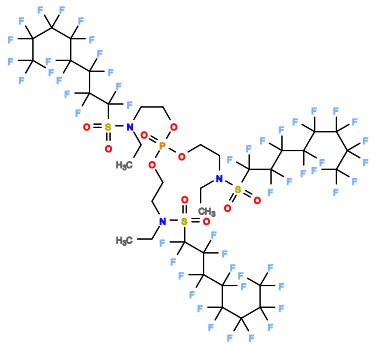
CAS RN	306973-47-7
Chemical Name	Sulfonamides, C4-8 -alkane, perfluoro, *N*-(hydroxyethyl)- *N*-methyl, reaction products with 12-hydroxystearic acid and 2,4 -TDI, ammonium salts

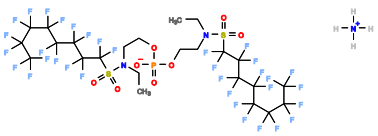
CAS RN	306975-56-4
Chemical Name	Propanoic acid, 3-hydroxy- 2-(hydroxymethyl) -2-methyl-, polymer with 2-ethyl -2-(hydroxymethyl) -1,3-propanediol and *N*, *N*', 2-tris(6-isocyanatohexyl) imidodicarbonic diamide reaction products with *N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8 heptadecafluoro-*N*-(2-hydroxyethyl)-1-octanesulfonamide and *N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-*N*-(2-hydroxyethyl)-1-heptanesulfonamide, compds. with triethylamine

Phosphate Esters of Perfluorooctanesulfonamides

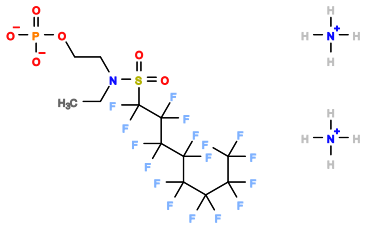
CAS RN	3820-83-5
Chemical Name	1-Octanesulfonamide, *N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-*N*-[2-(phosphonooxy)ethyl]-
Synonyms	*N*-ethyl perfluorooctanesulfonamidoethyl dihydrogen phosphate
Structural Formula	
Molecular Formula	$C_{12}H_{11}F_{17}NO_6PS$
Molecular Weight (g/mol)	651.23
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOP(=O)(O)O)CC

CAS RN	2250-98-8
Chemical Name	1-Octanesulfonamide, *N*,*N*',*N*''-[phosphinylidynetris(oxy-2,1-ethanediyl)]tris[*N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-
Synonyms	tris(*N*-ethyl perfluorooctanesulfonamidoethyl)phosphate

Structural Formula	
Molecular Formula	$C_{36}H_{27}F_{51}N_3O_{10}PS_3$
Molecular Weight (g/mol)	1757.70
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOP(=O)(OCCN(CC)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)OCCN(CC)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)CC

CAS RN	30381-98-7
Chemical Name	1-Octanesulfonamide, *N*,*N*'-[phosphinicobis(oxy-2,1-ethanediyl)]bis[*N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-, ammonium salt
Synonyms	ammonium bis(*N*-ethylperfluorooctanesulfonamidoethyl)phosphate
Structural Formula	
Molecular Formula	$C_{24}H_{22}F_{34}N_3O_8PS_2$
Molecular Weight (g/mol)	1221.50

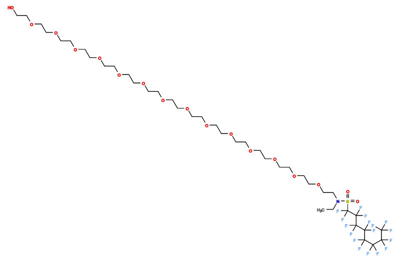
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F) C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOP(=O)([O-])OCCN(CC)S(=O)(=O)C(F) (F)C(F)(F)C(F)(F) C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)CC.[NH4+]

CAS RN	67969-69-1
Chemical Name	1-Octanesulfonamide, *N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-*N*-[2-(phosphonooxy)ethyl]-, diammonium salt
Synonyms	diammonium *N*-ethylperfluorooctanesulfonamidoethyl phosphate
Structural Formula	
Molecular Formula	$C_{12}H_{17}F_{17}N_3O_6PS$
Molecular Weight (g/mol)	685.29
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F) C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOP(=O)([O-])[O-])CC.[NH4+].[NH4+]

Polyglycol Derivatives of Perfluorooctanesulfonamides

The substance represented by CAS RN 29117-08-6 is reported to contain 14 ethylene glycol units (Huawen and Vijayendran, 2001).

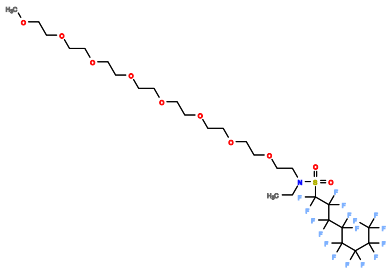
CAS RN	29117-08-6

Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-[2-[ethyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl]-.omega.-hydroxy-
Synonyms	*N*-ethylperfluorooctanesulfonamide poly(ethylene glycol)
Structural Formula	
Molecular Formula	$C_{40}H_{66}F_{17}NO_{17}S$
Molecular Weight (g/mol)	1187.99
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO)CC

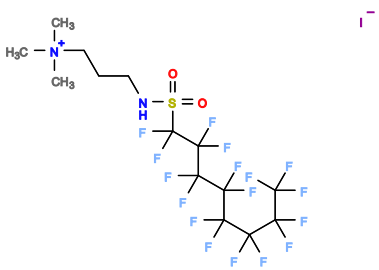
CAS RN	37338-48-0
Chemical Name	Poly[oxy(methyl-1,2-ethanediyl)], .alpha.-[2-[ethyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl]-.omega.-hydroxy-

The substance represented by CAS RN 68958-61-2 is a mixture of discrete chemicals. Representative chemical identity information is provided. However, it should be noted that this substance is expected to include a mixture of chemicals with polyethylene glycol chains containing between five and ten ethylene glycol units (average = 7.4) (Zou and Barton, 1994).

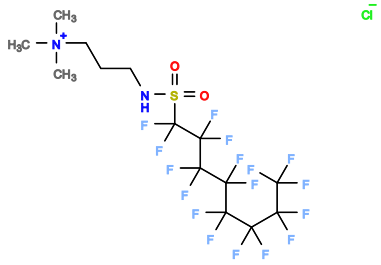
CAS RN	68958-61-2
Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-[2-[ethyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl]-.omega.-methoxy-

Synonyms	*N*-ethylperfluorooctanesulfonamidoethyl poly(ethylene glycol) methyl ether
Representative Structural Formula	
Representative Molecular Formula	$C_{27}H_{40}F_{17}NO_{10}S$
Representative Molecular Weight (g/mol)	893.65
Representative SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOCCOCCOCCOCCOCCOCCOCCOCCOC)CC

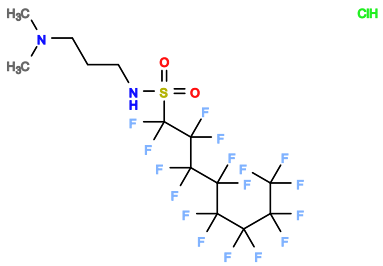
Alkyl Ammonium and Amine Derivatives of Perfluorooctanesulfonamides

CAS RN	1652-63-7
Chemical Name	1-Propanaminium, 3-[[(heptadecafluorooctyl)sulfonyl]amino]-*N*,*N*,*N*-trimethyl-, iodide
Synonyms	*N*-(3-(trimethyl)aminopropyl)perfluorooctanesulfonamide iodide
Structural Formula	

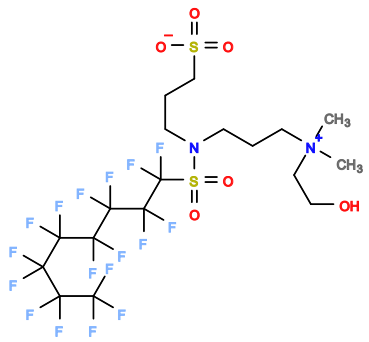
Molecular Formula	$C_{14}H_{16}F_{17}IN_2O_2S$
Molecular Weight (g/mol)	726.23
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)NCCC[N+](C)(C)C.[I-]

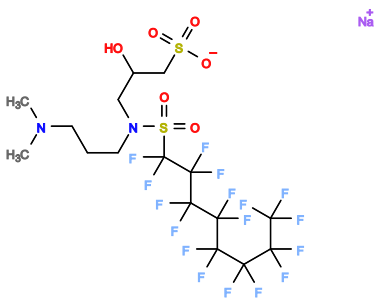
CAS RN	38006-74-5
Chemical Name	1-Propanaminium, 3-[[(heptadecafluorooctyl)sulfonyl]amino]-*N*,*N*,*N*-trimethyl-, chloride
Synonyms	*N*-(3-(trimethyl)aminopropyl)perfluorooctanesulfonamide chloride
Structural Formula	
Molecular Formula	$C_{14}H_{16}ClF_{17}N_2O_2S$
Molecular Weight (g/mol)	634.78
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)NCCC[N+](C)(C)C.[Cl-]

CAS RN	67939-88-2

Chemical Name	1-Octanesulfonamide, *N*-[3-(dimethylamino)propyl]-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-, monohydrochloride
Synonyms	*N*-(3-(dimethyl)aminopropyl)perfluorooctanesulfonamide monohydrochloride
Structural Formula	
Molecular Formula	$C_{13}H_{14}ClF_{17}N_2O_2S$
Molecular Weight (g/mol)	620.75
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)NCCCN(C)C.Cl

CAS RN	68298-11-3
Chemical Name	1-Propanaminium, 3-[[(heptadecafluorooctyl)sulfonyl](3-sulfopropyl)amino]-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-, hydroxide, inner salt
Synonyms	*N*-(3-(dimethyl)(hydroxyethyl)aminopropyl) perfluorooctanesulfonamide propylsulfonate, inner salt
Structural Formula	

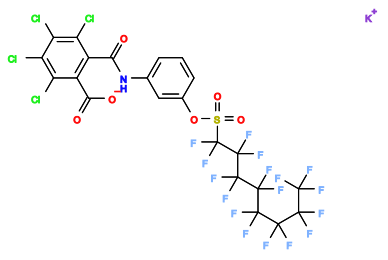
	
Molecular Formula	$C_{18}H_{23}F_{17}N_2O_6S_2$
Molecular Weight (g/mol)	750.49
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCC[N+](C)(C)CCO)CCCS(=O)(=O)[O-]

CAS RN	94133-90-1
Chemical Name	1-Propanesulfonic acid, 3-[[3-(dimethylamino)propyl][(heptadecafluorooctyl)sulfonyl]amino]-2-hydroxy-, monosodium salt
Synonyms	sodium *N*-(3-(dimethyl)aminopropyl) perfluorooctanesulfonamide 2-hydroxypropylsulfonate
Structural Formula	
Molecular Formula	$C_{16}H_{18}F_{17}N_2NaO_6S_2$

Molecular Weight (g/mol)	744.42
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CC(O)CS(=O)(=O)[O-])CCCN(C)C.[Na+]

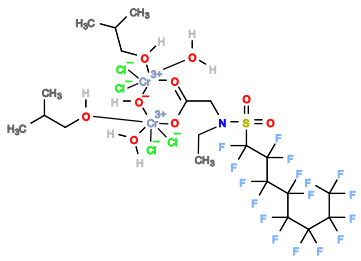
CAS RN	94133-91-2
Chemical Name	1-Propanaminium, 3-[[(heptadecafluorooctyl)sulfonyl](2-hydroxy-3-sulfopropyl)amino]-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-, hydroxide, monosodium salt

Miscellaneous Perfluorooctanesulfonyl Derivatives

CAS RN	57589-85-2
Chemical Name	Benzoic acid, 2,3,4,5-tetrachloro-6-[[[3-[[(heptadecafluorooctyl)sulfonyl]oxy]phenyl]amino]carbonyl]-, monopotassium salt
Synonyms	potassium 2,3,4,5-tetrachloro-6-[[[3-[[perfluorooctanesulfonyl]oxy]phenyl]amino]carbonyl] benzoate
Structural Formula	
Molecular Formula	$C_{22}H_5Cl_4F_{17}KNO_6S$
Molecular Weight (g/mol)	915.22

SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)Oc1cc(NC(=O)c2c(C(=O)[O-])c(Cl)c(Cl)c(Cl)c2Cl)ccc1.[K+]

The substance represented by CAS RN 68891-96-3 is a dinuclear coordination complex of chromium. The chromium ions in this complex are present in the 3+ oxidation state.

CAS RN	68891-96-3
Chemical Name	Chromium, diaquatetrachloro[.mu.-[*N*-ethyl-*N*-[(heptadecafluorooctyl)sulfonyl]glycinato-O1:O1']]-.mu.-hydroxybis[2-methylpropanol]di-
Synonyms	*N*-ethylperfluorooctanesulfonylamido acetate chromium complex
Structural Formula	
Molecular Formula	$C_{20}H_{32}Cl_4Cr_2F_{17}NO_9S$
Molecular Weight (g/mol)	1031.31
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CC1O[Cr+++]([OH]CC(C)C)([OH2])([Cl-])([Cl-])[OH-][Cr+++]([OH2])([OH]CC(C)C)([Cl-])([Cl-])O=1)CC

CAS RN	944578-05-6

Chemical Name	Sulfonamides, C4-8-alkane, perfluoro, *N*-[4,7-dimethyl-4-[[(1-methylpropylidene)amino]oxy]-3,5-dioxa-6-aza-4-silanon-6-en-1-yl]-*N*-ethyl

Physical and Chemical Properties

Limited measured physical and chemical property data are available for the chemicals in this group.

The substances in this group include a wide range of neutral and ionic organic chemicals, polymers, telomers, UVCBs, and a coordination complex. Based on the available data, all are expected to be solids under ambient conditions (Hekster, et al., 2002; LMC, 2013). The higher molecular weight chemicals, including the telomers, polymers, and the chromium coordination complex are all expected to be involatile. However, the relatively lower molecular weight neutral organic substances may be volatile. Data available for EtFOSE indicate moderate volatility, with a measured vapour pressure of 0.504 Pa (Hekster, et al., 2002).

The measured water solubility value available for EtFOSE (0.151 mg/L) indicates that some chemicals in this group may be slightly soluble in water (Hekster, et al., 2002). When considered alongside volatility data, these values suggest some chemicals in this group may be moderately volatile from water (for example, estimated Henry's law constant for EtFOSE = 58 Pa-m^3/mol) (US EPA, 2008).

Import, Manufacture and Use

Australia

No Australian manufacture or export of PFOS related chemicals is known (NICNAS, 2018b; Parliament of Australia, 2014). No import data specific to the individual chemicals in this group have been identified.

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

International

Due to their unique chemical properties, perfluorinated chemicals have found use in a wide range of industrial applications. In the early 2000s, it was estimated that almost 500 tonnes of PFOS-based chemicals were used in the EU per annum, with significant uses including fabric treatments (49%), paper treatments (33%) and coating products, such as paints (18%) (Brooke, et al., 2004). However, use of PFOS containing chemicals has been declining globally. Concerns regarding persistence and bioaccumulation resulted in the largest global manufacturer of PFOS-based chemicals ceasing production of these chemicals in 2002 (3M, 2014; OECD, 2002). Nevertheless, production by various additional companies increased shortly after the phase out by the main manufacturer (US EPA, 2009).

Available data indicate that the chemicals in this group have multiple specialised applications. While the alcohols (e.g. EtFOSE and MeFOSE) and phosphate esters in this group have traditionally been used in fabric and paper treatments, more recent uses appear to predominantly be in paints, lacquers and varnishes (Hekster, et al., 2002; INERIS, 2013; Nordic Council of Ministers, 2015). In 2010, MeFOSE was reported to have been used in over 40 products in two Nordic countries (Nordic Council of Ministers, 2015).

The acetate salt (CAS RN 2991-51-7) and polyglycols (e.g. CAS RNs 29117-08-6 and 68958-61-2) have previously been used in industrial surfactant formulations (Flick, 1993). Use of the acetate has recently been reported in surface treatments, cleaning products and floor waxes (Nordic Council of Ministers, 2015). The alkyl ammonium derivatives are expected to have similar uses, with use of the quaternary ammonium salt (CAS RN 1652-63-7) reported in various Nordic countries in 2012 (Nordic Council of Ministers, 2015).

The reactive acrylate, EtFOSAC (CAS RN 423-82-5), and methacrylate, EtFOSMAC (CAS RN 376-14-7), are both expected to be used primarily as monomers in the manufacture of polymers and telomers (Buck, et al., 2011; Klun, et al., 2008; Smith, 1997). Use of a number of the resultant polymers and telomers has been reported recently. One acrylate polymer (CAS RN 68298-62-4) was reported to be present in over 70 preparations across two Nordic countries in 2012, with the majority being paint and coating products for motor vehicle bodywork. Other polymers and telomers are expected to have uses as impregnation agents (particularly in textiles), with one polymer (CAS RN 68555-92-0) identified as being used for this purpose in two Nordic countries in 2012 (KEMI, 2006; Nordic Council of Ministers, 2015).

Environmental Regulatory Status

Australia

In accordance with regulation 11C(1) under the *Industrial Chemicals (Notification and Assessment) Regulations 1990* (Cwlth), introduction or export of chemicals listed on the Rotterdam Convention is prohibited unless approval is obtained from the NICNAS Director (Commonwealth of Australia, 1990).

In 2008, a factsheet published by NICNAS recommended that PFOS-based chemicals be restricted to essential uses only, and that importers ensure that alternative chemicals are less toxic and not persistent in the environment (NICNAS, 2018b).

United Nations

Perfluorooctanesulfonic acid, perfluorooctanesulfonates, perfluorooctanesulfonamides and perfluorooctanesulfonyls are listed on Annex III of the Rotterdam Convention (UNEP, 2013). The Rotterdam Convention aims to facilitate sharing of chemical information to promote shared responsibility for the international trade of certain hazardous chemicals. Of the 193 United Nations member countries, 153 have ratified the Rotterdam Convention, including Australia. The European Union is also a party to the convention (UNEP, 2014).

The chemicals in this group are not currently identified as Persistent Organic Pollutants (UNEP, 2001) or ozone depleting substances (UNEP, 1987).

OECD

The chemicals in this group have not been identified as High Production Volume chemicals, or sponsored for assessment under the Cooperative Chemicals Assessment Programme (OECD, 2013).

Canada

Chemicals containing the PFOS moiety, including neutral and ionic organic chemicals, polymers, telomers and UVCBs, are listed under Schedule 1 (the Toxic Substances List) of the *Canadian Environmental Protection Act 1999*. The import, manufacture, sale and use of these chemicals are prohibited, unless destined for an exempted application. Such applications include certain uses in photolithography, in aviation hydraulic fluid, as fume suppressants and in aqueous film forming foam at concentrations less than 0.5 parts per million (Government of Canada, 2008).

The majority of the chemicals in this group are not listed on the Canadian Domestic Substances List (DSL) (Government of Canada, 2013). The 13 chemicals which are listed were found to be Persistent (P) and Inherently Toxic to the Environment (iT_E) during the Categorization of the DSL. Two polymers (CAS RNs 68329-56-6 and 70776-36-2) and the chromium complex (CAS RN 68891-96-3) were found to be Not Bioaccumulative (Not B), while the two quaternary ammonium surfactants (CAS RNs 1652-63-7 and 38006-74-5), two simple sulfonamide alcohols (CAS RNs 24448-09-7 and 1691-99-2) and an alcohol phosphate derivative (CAS RN 67969-69-1) were found to be Bioaccumulative (B). The bioaccumulation potentials of the remaining chemicals on the DSL were unable to be determined (Environment and Climate Change Canada, 2019).

European Union

The use of chemicals containing the PFOS moiety, including neutral and ionic organic chemicals, polymers, telomers and UVCBs, is restricted under Commission Regulation No 850/2004 on Persistent Organic Pollutants (European Commission, 2010). These chemicals may only be used in select applications in electroplating systems, photolithography processes, photographic coatings, chromium plating, and aviation hydraulic fluids. Use is to be phased out as alternate substances or technologies become available.

Twenty-seven chemicals in this group have been pre-registered for use in the European Union under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation (ECHA, 2015). However, no chemicals in this group have yet undergone the full registration process (ECHA, 2014).

United States of America

Forty-five chemicals in this group, including neutral and ionic organic chemicals, polymers, telomers and UVCBs, are listed on the inventory of chemicals manufactured or processed in the USA, as published under the *Toxic Substances Control Act 1976* (US EPA, 2014). All chemicals listed are subject to Significant New Use Rules. Approval is required before any of these chemicals may be used for any new applications as outlined under Section 721.9582 of the *Code of Federal Regulations* (US EPA, 2011).

The United States Environmental Protection Agency (US EPA) published an action plan on long-chain perfluorinated chemicals, covering the chemicals in this group, in 2009. All chemicals were identified as persistent, bioaccumulative and toxic (US EPA, 2009).

Environmental Exposure

Based on international use pattern information, chemicals in this group may have industrial uses in Australia. Release to the environment may occur during the use and disposal of formulations containing these chemicals.

The environmental degradant of primary concern for the chemicals in this group is PFOS. Biodegradation data available for EtFOSE demonstrate conversion to the corresponding carboxylic acid, *N*-ethylperfluorooctanesulfonamidoacetic acid (EtFOSAA), with the ultimate biodegradation product being PFOS (Hekster, et al., 2002; Martin, et al., 2010). This perfluorinated anion is purely of anthropogenic origin and has been identified as a POP under the Stockholm Convention (NICNAS, 2015a). It is widely assumed that analogous perfluorosulfonamides will be susceptible to similar biotransformation processes (Martin, et al., 2010).

Studies conducted with the shorter-chain perfluorobutanesulfonate homologue of MeFOSE also indicate potential for atmospheric degradation to PFOS. Oxidation by hydroxyl radicals was found to produce traces of the sulfonate, as well as aldehyde, sulfonamide and carboxylic acid derivatives. However, detailed information on the yield is not available (D'eon, et al., 2006; Martin, et al., 2010).

Monitoring data have identified some of the chemicals in this group and their degradation products in the environment. The two volatile alcohols (MeFOSE and EtFOSE) are routinely detected in outdoor air. Highest concentrations were found in air sampling conducted in Toronto, Canada in 2001, with the chemicals found in mean concentrations of 1.0×10^{-4} micrograms per cubic metre ($\mu g/m^3$) and $2.1 \times 10^{-4} \mu g/m^3$, respectively (Martin, et al., 2010). In surface water, EtFOSAA has been measured at concentrations up to 7.5 nanograms per litre (ng/L) (Martin, et al., 2010).

Further, PFOS has been found to be a widely distributed environmental pollutant. International studies have identified PFOS in various environmental media, including surface and drinking waters. In Australia, PFOS has been found in drinking water at concentrations up to 16 ng/L (Thompson, et al., 2011). However, it is noted there are multiple potential sources of PFOS in the environment, including past industrial use of direct precursors to PFOS or use of PFOS-related substances in articles, in addition to the industrial use of derivatives of PFOS which degrade to this substance in the environment.

Environmental Effects

No ecotoxicity data were located for the parent chemicals in this group.

The currently available ecotoxicity data for PFOS are summarised in the IMAP-Environment Tier II assessment of Direct Precursors to PFOS. Data currently available for PFOS indicate moderate acute aquatic toxicity (median lethal/effective concentration values = 3.6-48.2 mg/L) and chronic toxicity (no-observed-effect concentration values = 0.25-7 mg/L) in standard ecotoxicity tests. However, data from a growing number of non-standard ecotoxicity tests have identified intergenerational toxicity in offspring when parent generations are exposed to concentrations as low as 0.01 mg/L (NICNAS, 2015a).

It is noted that the chemicals in this group contain a range of functional groups and moieties which are correlated with acute toxic effects in aquatic organisms. However, these possible effects have not been considered in this assessment, as the primary risk posed by the chemicals in this group is assumed to result from the cumulative release of PFOS into the environment.

Categorisation of Environmental Hazard

Insufficient data are presented in this assessment to categorise the chemicals in this group according to domestic environmental hazard thresholds (EPHC, 2009).

It is noted that direct precursors to PFOS are categorised as Persistent, Bioaccumulative and Toxic (PBT) substances according to domestic environmental hazard criteria (NICNAS, 2015a).

Risk Characterisation

The chemicals in this group may degrade to a PBT substance. It is not currently possible to derive a safe environmental exposure level for such chemicals and it is therefore not appropriate to characterise the environmental risks for these chemicals in terms of a risk quotient.

The recalcitrant degradant assumed to be formed from each of the chemicals in this group (PFOS) has been identified as a POP under the Stockholm Convention. Persistent Organic Pollutants are chemical substances that persist in the environment, bioaccumulate in humans and wildlife, undergo long-range transport to regions where they have never been used or produced, and pose a risk of causing harmful effects on human health and the environment. The international community has now, on several occasions, called for urgent global actions to reduce and/or eliminate production and use of such chemicals.

Key Findings

Based on international data, chemicals in this group may have current industrial use in Australia in a range of products.

Available environmental degradation data show that some chemicals in this group degrade to PFOS. Therefore, the principal risk posed by the chemicals in this group if emitted to the environment has been assumed to result from the cumulative releases of PFOS. This perfluorinated chemical has been identified as a POP under the Stockholm Convention.

The chemicals in this group have not been categorised according to domestic environmental hazard criteria. This finding does not indicate a lack of potential hazard for some parent chemicals in this group, but rather a lack of suitable data to characterise these hazards for each individual chemical.

The assessment of the risks from these chemicals to human health, including public health, has been considered in the IMAP-Human Health Tier II assessment for Indirect Precursors to Perfluorooctanesulfonate (PFOS) (NICNAS, 2015b).

Recommendations

The chemicals in this group have been assessed as having the potential to give rise to adverse outcomes for the environment and public health. These chemicals are currently listed on the Australian Inventory of Chemical Substances (the Inventory), and are available to be introduced into Australia without any further assessment by NICNAS. Other chemicals with reduced potential for adverse outcomes are becoming available but, given the properties of these chemicals, their assessment as new chemicals

under the *Industrial Chemicals (Notification and Assessment) Act 1989* (the ICNA Act) is still required to fully characterise the human health and the environmental risks associated with their use.

It is recommended that NICNAS consult with industry and other stakeholders to consider strategies, including regulatory mechanisms available under the ICNA Act, to encourage the use of safer chemistry.

Environmental Hazard Classification

Insufficient data are presented in this assessment to classify the aquatic hazards of chemicals in this group according to the third edition of the United Nations' Globally Harmonised System of Classification and Labelling of Chemicals (GHS) (UNECE, 2009).

It is noted that direct precursors to PFOS have been classified as Acute Aquatic Category 2 (H401) and Chronic Aquatic Category 1 (H410) under the GHS (NICNAS, 2015a).

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