Indirect precursors to perfluorocarboxylic acids: Environment tier II assessment

12 December 2019

CAS Registry Numbers: 865-86-1, 39239-77-5, 68391-08-2, 2144-54-9, 6014-75-1, 4980-53-4, 59778-97-1, 65104-66-7, 85631-54-5, 65605-58-5, 65605-59-6, 65605-60-9, 65636-35-3, 68239-43-0, 150135-57-2, 203743-03-7, 65104-45-2, 115592-83-1, 119973-85-2, 196316-34-4, 125768-41-4, 220237-52-5, 65530-83-8, 65530-69-0, 65530-59-8, 65605-57-4, 65605-56-3, 94095-37-1, 71608-61-2, 68891-05-4, 376364-33-9, 135228-60-3, 144468-32-6, 118102-37-7, 118102-38-8, 332076-28-5, 332076-33-2, 332076-34-3, 68990-40-9, 253873-70-0, 65530-74-7, 65530-63-4, 65530-64-5, 74499-44-8, 65545-80-4, 70983-59-4, 98219-29-5, 115340-82-4, 92129-34-5, 115535-36-9, 127133-57-7, 145477-02-7, 153325-45-2, 65530-57-6, 71002-41-0, 68187-47-3, 68187-25-7, 70983-60-7, 71356-38-2, 68140-21-6, 68516-17-6, 84238-62-0, 70969-47-0, 113089-67-1, 253682-98-3, 253682-97-2, 185630-70-0, 459415-06-6, 524729-93-9, 1094598-90-9, 325966-78-7, 119973-84-1, 220713-37-1, 374928-93-5, 97136-02-2, 101896-32-6, 220713-74-6, 220713-85-9, 374928-92-4, 329201-80-1, 65530-58-7, 254889-79-7, 254889-72-0, 500701-62-2, 428842-38-0, 59493-72-0

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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

NICNAS has made every effort to assure the quality of information available in this report. However, before relying on it for a specific purpose, users should obtain advice relevant to their particular circumstances. This report has been prepared by NICNAS using a range of sources, including information from databases maintained by third parties, which include data supplied by industry. NICNAS has not verified and cannot guarantee the correctness of all information obtained from those databases. Reproduction or further distribution of this information may be subject to copyright protection. Use of this information without obtaining the permission from the owner(s) of the respective information might violate the rights of the owner. NICNAS does not take any responsibility whatsoever for any copyright or other infringements that may be caused by using this information.

Grouping Rationale

This Tier II assessment considers the environmental risks associated with the industrial uses of a group of 86 fluorochemicals. The chemicals in this group include neutral and ionic organic substances of moderate to high molecular weight, and polymers with fluorinated side-chains. All but one of the substances in this group contain a chain of perfluorinated carbons that are linked to another structural unit by at least one non-fluorinated carbon atom. Although some substances in this group are mixtures of

discrete chemicals with a range of perfluorinated chain lengths, all potentially have at least one component chemical which has a chain of nine or more perfluorinated carbon atoms.

NICNAS has developed an action plan to assess and manage chemicals which may degrade to perfluorinated carboxylic acids (PFCAs), perfluoroalkyl sulfonates and similar chemicals (NICNAS, 2018). The primary assumption outlined in this action plan is that chemicals with a perfluorinated carbon chain terminated with an alkyl or aryl group will degrade to form a mix of perfluorocarboxylic acids, with both the original perfluorinated chain length and one less perfluorinated carbon atom.

The environmental biodegradation of chemicals in this group is expected to primarily result in release of perfluorocarboxylic acids with one less perfluorinated carbon atom than the parent chemical. On this basis, the chemicals in this group are considered to have the potential to degrade to perfluorononanoic acid and/or a longer chain perfluorocarboxylic acid homologue. These potential long-chain perfluorocarboxylic acid degradants are of concern because the immediate shorter chain homologue, perfluorooctanoic acid (PFOA), has been identified as a persistent, bioaccumulative and toxic (PBT) chemical according to domestic environmental hazard criteria. Chemicals with these hazard characteristics are of high concern to the environment and PFOA (and substances which may degrade to PFOA) are subject to increasingly stringent regulatory controls in other developed countries (NICNAS, 2015a).

Longer chain perfluorocarboxylic acids have received attention internationally for similar reasons. In 2009, long-chain perfluorocarboxylic acids were identified as PBT substances in the United States of America (USA) (US EPA, 2009). Canada has prohibited the introduction of long-chain perfluorocarboxylic acids and their precursors (Government of Canada, 2018b). A series of long-chain perfluorocarboxylic acids has also been identified as Substances of Very High Concern in the European Union due to their very persistent and very bioaccumulative (vPvB) hazard characteristics (ECHA, 2012a, b, c, d).

The degradation of perfluorinated carboxylic acids is very slow compared with their rate of formation from degradation of the precursors and perfluorinated carboxylic acids will be the final degradants from multiple precursors. Therefore, the amount of perfluorinated carboxylic acids 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 release of perfluorinated carboxylic acids to the environment.

Chemical Identity

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).

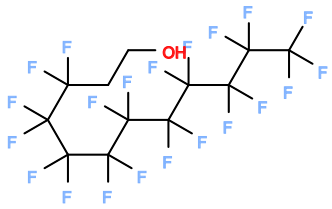
This assessment includes a range of neutral and ionic organic chemicals, polymers, and chemicals that are in the category of unknown or variable composition, complex reaction products or biological materials (UVCBs). The chemicals in this assessment have been sub-grouped based on similar structural properties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

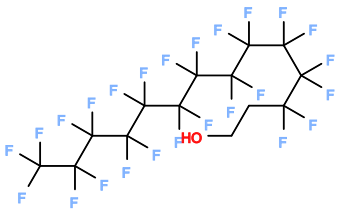
Structural information is presented where it is available. For polymers, constituent monomers are presented. Due to the typically variable size and structure of polymer molecules, the molecular formula and molecular weight for these substances are not presented.

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

Neutral Organic Derivatives of Fluorotelomer Alcohols

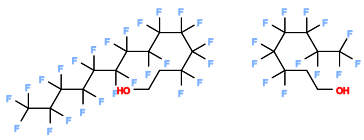
CAS RN	865-86-1
Chemical Name	1-Dodecanol, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluoro-

Synonyms	10:2 FTOH 10:2 fluorotelomer alcohol
Structural Formula	
Molecular Formula	$C_{12}H_5F_{21}O$
Molecular Weight	564.13
SMILES	C(F)(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)C(F)(F)C(F)(F)CCO

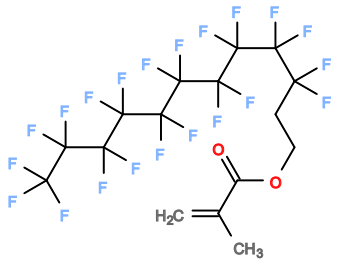
CAS RN	39239-77-5
Chemical Name	1-Tetradecanol, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluoro-
Synonyms	12:2 FTOH 12:2 fluorotelomer alcohol
Structural Formula	
Molecular Formula	$C_{14}H_5F_{25}O$
Molecular Weight	664.15

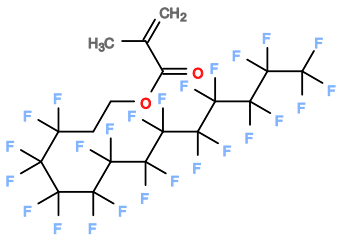
SMILES	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCO

The substance represented by CAS RN 68391-08-2 is a UVCB. Representative chemical identity information is provided for the two end members of this substance below. This substance is a mixture of fluorotelomer alcohols with chains of six to twelve perfluorinated carbons.

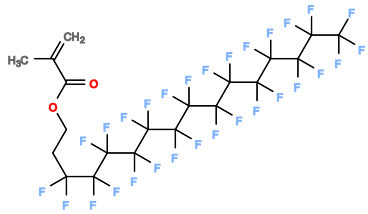
CAS RN	68391-08-2
Chemical Name	Alcohols, C8-14, .gamma.-.omega.-perfluoro
Representative Structural Formula	
Representative Molecular Formula	$C_8H_5F_{13}O$ $C_{14}H_5F_{25}O$
Representative Molecular Weight (g/mol)	364.10 664.15
Representative SMILES	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCO C(F)(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)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCO

CAS RN	2144-54-9
Chemical Name	2-Propenoic acid, 2-methyl-, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluorododecyl ester
Synonyms	10:2 FTMAC 10:2 fluorotelomer methacrylate

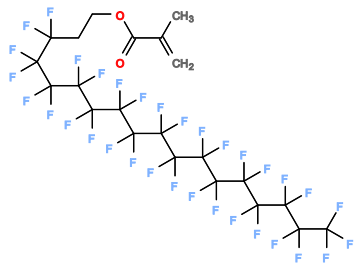
Structural Formula	
Molecular Formula	$C_{16}H_9F_{21}O_2$
Molecular Weight	632.21
SMILES	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCOC(=O)C(=C)C

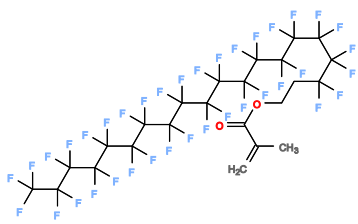
CAS RN	6014-75-1
Chemical Name	Methacrylic acid, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecyl ester
Synonyms	12:2 FTMAC 12:2 fluorotelomer methacrylate
Structural Formula	
Molecular Formula	$C_{18}H_9F_{25}O_2$
Molecular Weight	732.22

SMILES	C(F)(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)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCOC(=O)C(=C)C

CAS RN	4980-53-4
Chemical Name	Methacrylic acid, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,15,15,16,16,16-nonacosafluorohexadecyl ester
Synonyms	14:2 FTMAC 14:2 fluorotelomer methacrylate
Structural Formula	
Molecular Formula	$C_{20}H_9F_{29}O_2$
Molecular Weight	832.24
SMILES	C(F)(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)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCOC(=O)C(=C)C

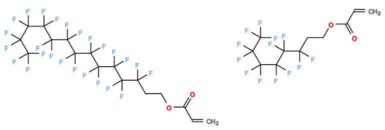
CAS RN	59778-97-1
Chemical Name	2-Propenoic acid, 2-methyl-, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,15,15,16,16,17,17,18,18,18-tritriacontafluorooctadecyl ester
Synonyms	16:2 FTMAC 16:2 fluorotelomer methacrylate

Structural Formula	
Molecular Formula	$C_{22}H_9F_{33}O_2$
Molecular Weight	932.25
SMILES	C(F)(F)(F)CCOC(=O)C(=C)C

CAS RN	65104-66-7
Chemical Name	2-Propenoic acid, 2-methyl-, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,15,15,16,16,17,17,18,18,19,19,20,20,20-heptatriacontafluoroeicosyl ester
Synonyms	18:2 FTMAC 18:2 fluorotelomer methacrylate
Structural Formula	
Molecular Formula	$C_{24}H_9F_{37}O_2$
Molecular Weight	1032.27

SMILES	C(F)(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)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCOC(=O)C(=C)C

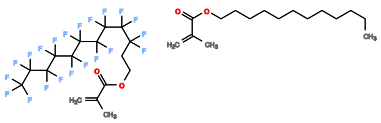
The substance represented by CAS RN 85631-54-5 is a UVCB. Representative chemical identity information is provided for the two end members of this substance below. This substance is a mixture of fluorotelomer acrylates with chains of six to twelve perfluorinated carbons.

CAS RN	85631-54-5
Chemical Name	2-Propenoic acid, .gamma.-.omega.-perfluoro-C8-14-alkyl esters
Representative Structural Formula	
Representative Molecular Formula	$C_{11}H_7F_{13}O_2$ $C_{17}H_7F_{25}O_2$
Representative Molecular Weight (g/mol)	418.15 718.20
Representative SMILES	C=CC(=O)OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)(F) C=CC(=O)OCCC(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)C(F)(F)C(F)(F)C(F)(F)(F)

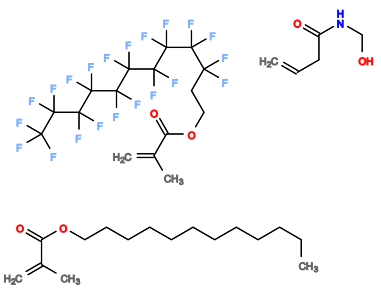
Methacrylate and Acrylate Polymers

The substance represented by CAS RN 65605-58-5 is a polymer with side chains terminated with perfluorinated segments of various lengths. Representative chemical identity information is provided for the constituent monomers below.

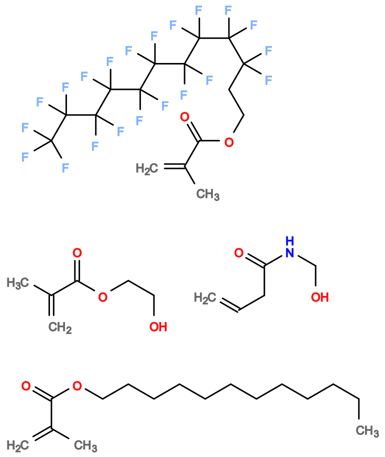
CAS RN	65605-58-5
Chemical Name	2-Propenoic acid, 2-methyl-, dodecyl ester, polymer with .alpha.-fluoro-.omega.-[2-[(2-methyl-1-oxo-2-

	propenyl)oxy]ethyl]poly(difluoromethylene)
Synonyms	dodecyl methacrylate, polymer with perfluoroalkylethyl methacrylate
Representative Structural Formula	
Representative SMILES	CCCCCCCCCCCCOC(=O)C(=C)C.C(F)(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)C(F)(F)C(F)(F)C(F)(F)CCOC(=O)C(=C)C

The substance represented by CAS RN 65605-59-6 is a polymer with side chains terminated with perfluorinated segments of various lengths. Representative chemical identity information is provided for the constituent monomers below.

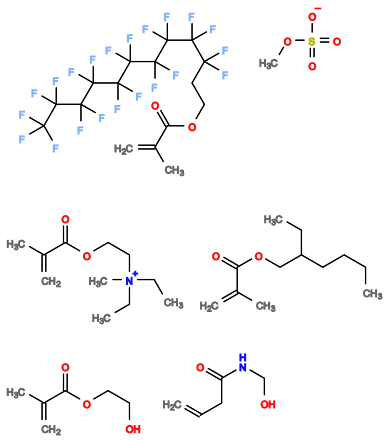
CAS RN	65605-59-6
Chemical Name	2-Propenoic acid, 2-methyl-, dodecyl ester, polymer with .alpha.-fluoro-.omega.-[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]poly(difluoromethylene) and *N*-(hydroxymethyl)-2-propenamide
Synonyms	dodecyl methacrylate, polymer with perfluoroalkylethyl methacrylate and *N*-hydroxymethylacrylamide
Representative Structural Formula	
Representative SMILES	CCCCCCCCCCCCOC(=O)C(=C)C.C(F)(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)C(F)(F)C(F)(F)C(F)(F)CCOC(=O)C(=C)C.OCNC(=O)CC(=C)

The substance represented by CAS RN 65605-60-9 is a polymer with side chains terminated with perfluorinated segments of various lengths. Representative chemical identity information is provided for the constituent monomers below.

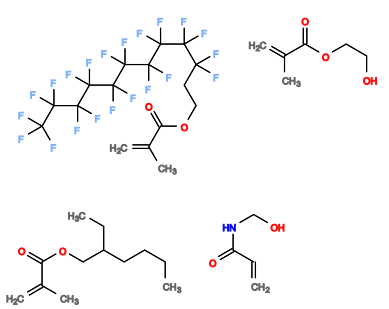
CAS RN	65605-60-9
Chemical Name	2-Propenoic acid, 2-methyl-, dodecyl ester, polymer with .alpha.-fluoro-.omega.-[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]poly(difluoromethylene), 2-hydroxyethyl 2-methyl-2-propenoate and *N*-(hydroxymethyl)-2-propenamide
Synonyms	dodecyl methacrylate, polymer with perfluoroalkylethyl methacrylate, 2-hydroxyethyl methacrylate and *N*-hydroxymethylacrylamide
Representative Structural Formula	
Representative SMILES	CCCCCCCCCCCCOC(=O)C(=C)C.C(F)(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)C(F)(F)CCOC(=O)C(=C)C.OCNC(=O)CC(=C).OCCOC(=O)C(C)=C

The substance represented by CAS RN 65636-35-3 is a polymer with side chains terminated with perfluorinated segments of various lengths. Representative chemical identity information is provided for the constituent monomers below.

CAS RN	65636-35-3
Chemical Name	Ethanaminium, *N*,*N*-diethyl-*N*-methyl-2-[(2-methyl-1-oxo-2-propenyl)oxy]-, methyl sulfate, polymer with 2-ethylhexyl 2-methyl-2-propenoate, .alpha.-fluoro-.omega.-[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]poly(difluoromethylene), 2-hydroxyethyl 2-methyl-2-propenoate and *N*-(hydroxymethyl)-2-propenamide
Synonyms	diethylaminoethyl methacrylate dimethyl sulphate, polymer with 2-ethylhexyl acrylate, perfluoroalkylethyl methacrylate, 2-hydroxyethyl methacrylate and *N*-

	hydroxymethylacrylamide
Representative Structural Formula	
Representative SMILES	CCCCC(CC)COC(=O)C(=C)C.C(F)(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)C(F)(F)C(F)(F)C(F)(F)CCOC(=O)C(=C)C.OCNC(=O)CC(=C).OCCOC(=O)C(C)=C.[N+](C)(CC)(CC)CCOC(=O)C(C)=C.S(=O)(=O)([O-])OC

The substance represented by CAS RN 68239-43-0 is a polymer with side chains terminated with perfluorinated segments of various lengths. Representative chemical identity information is provided for the constituent monomers below.

CAS RN	68239-43-0
Chemical Name	2-Propenoic acid, 2-methyl-, 2-ethylhexyl ester, polymer with .alpha.-fluoro-.omega.-[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]poly(difluoromethylene), 2-hydroxyethyl 2-methyl-2-propenoate and *N*-(hydroxymethyl)-2-propenamide
Synonyms	2-ethylhexyl acrylate, polymer with perfluoroalkylethyl methacrylate, 2-hydroxyethyl methacrylate and *N*-hydroxymethylacrylamide
Representative Structural Formula	
Representative SMILES	OCCOC(=O)C(=C)C.CCCCC(CC)COC(=O)C(=C)C.OCNC(=O)C(=C).C(F)(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)C(F)(F)C(F)(F)C(F)(F)CCOC(=O)C(=C)C

CAS RN	150135-57-2
Chemical Name	2-Propenoic acid, 2-methyl-, 2-(dimethylamino)ethyl ester, polymers with Bu acrylate, gamma-omega-perfluoro-C8-14-alkyl acrylate and polyethylene glycol monomethacrylate, 2,2'-azobis[2,4-dimethylpentanenitrile]-initiated

CAS RN	203743-03-7
Chemical Name	2-Propenoic acid, 2-methyl-, hexadecyl ester, polymers with 2-hydroxyethyl methacrylate, .gamma.-.omega.-perfluoro-C10-16-alkyl acrylate and stearyl methacrylate

CAS RN	65104-45-2
Chemical Name	2-Propenoic acid, 2-methyl-, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluorododecyl ester, polymer with 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl 2-methyl-2-propenoate, methyl 2-methyl-2-propenoate, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecyl 2-methyl-2-propenoate and 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl 2-methyl-2-propenoate

CAS RN	115592-83-1
Chemical Name	2-Propenoic acid, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluorododecyl ester, polymer with 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl 2-propenoate, hexadecyl 2-propenoate, *N*-(hydroxymethyl)-2-propenamide, octadecyl 2-propenoate, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecyl 2-propenoate and 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl 2-propenoate

CAS RN	119973-85-2
Chemical Name	2-Propenoic acid, 2-methyl-, 3-chloro-2-hydroxypropyl ester, polymer with 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluorododecyl 2-propenoate, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl 2-propenoate, *N*-(hydroxymethyl)-2-propenamide, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,15,15,16,16,16-nonacosafluorohexadecyl 2-propenoate, octadecyl 2-propenoate and 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecyl 2-propenoate

CAS RN	196316-34-4
Chemical Name	2-Propenoic acid, 2-methyl-, 2-(dimethylamino)ethyl ester, polymers with .gamma.-.omega.-perfluoro-C10-16-alkyl acrylate and vinyl acetate, acetates

CAS RN	1094598-90-9
Chemical Name	2-Propenoic acid, 2-methyl-, 3-chloro-2-hydroxypropyl ester, polymer with 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluorododecyl 2-propenoate, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl 2-propenoate, *N*-(hydroxymethyl)-2-propenamide, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,15,15,16,16,16-nonacosafluorohexadecyl 2-propenoate, octadecyl 2-propenoate, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecyl 2-propenoate and 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl 2-propenoate

CAS RN	325966-78-7
Chemical Name	2-Propenoic acid, 2-methyl-, 3-chloro-2-hydroxypropyl ester, polymers with *N*-(1,1-dimethyl-3-oxobutyl)-2-propenamide, 2-ethylhexyl acrylate, gamma-omega-perfluoro-C8-16-alkyl acrylate, octadecyl 2-propenoate and vinyl chloride, 2,2'-azobis[2-methylpropanimidamide] dihydrochloride-initiated

CAS RN	119973-84-1

Chemical Name	2-Propenoic acid, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluorododecyl ester, polymer with 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl 2-propenoate, alpha.-(2-methyl-1-oxo-2-propenyl)-omega.-[(2-methyl-1-oxo-2-propenyl)oxy]poly(oxy-1,2-ethanediyl), 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,15,15,16,16,16-nonacosafluorohexadecyl 2-propenoate, octadecyl 2-propenoate and 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecyl 2-propenoate

CAS RN	220713-37-1
Chemical Name	2-Propenoic acid, 2-methyl-, 2-aziridinyl ester, polymer with alpha-fluoro-omega-[2-[(1-oxo-2-propenyl)oxy]ethyl]poly(difluoromethylene) and phenylmethyl 2-methyl-2-propenoate

CAS RN	374928-93-5
Chemical Name	2-Propenenitrile, polymer with .alpha.-fluoro-.omega.-[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]poly(difluoromethylene), .alpha.-(2-methyl-1-oxo-2-propenyl)-.omega.-methoxypoly(oxy-1,2-ethanediyl) and .alpha.-(2-methyl-1-oxo-2-propenyl)-.omega.-[(2-methyl-1-oxo-2-propenyl)oxy]poly(oxy-1,2-ethanediyl)

CAS RN	97136-02-2
Chemical Name	2-Propenoic acid, 2-methyl-, 2-ethylhexyl ester, polymer with .alpha.-fluoro-.omega.-[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]poly(difluoromethylene)

CAS RN	101896-32-6
Chemical Name	2-Propenoic acid, 2-methyl-, 3-chloro-2-hydroxypropyl ester, polymer with .alpha.-fluoro-.omega.-[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]poly(difluoromethylene)

CAS RN	220713-74-6
Chemical Name	2-Propenoic acid, 2-methyl-, 2-aziridinyl ester, polymer with alpha-fluoro-omega-[[(2-methyl-1-oxo-2-propenyl)oxy]methyl]poly(difluoromethylene) and octadecyl 2-methyl-2-propenoate

CAS RN	220713-85-9
Chemical Name	2-Propenoic acid, 2-methyl-, 2-aziridinyl ester, polymer with 1,1-dimethylethyl 2-methyl-2-propenoate and alpha-fluoro-omega-[[(2-methyl-1-oxo-2-propenyl)oxy]methyl]poly(difluoromethylene)

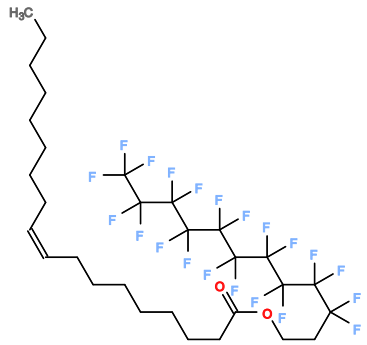
CAS RN	374928-92-4
Chemical Name	2-Butenedioic acid (2Z)-, dioctyl ester, polymer with chloroethene and alpha-fluoro-omega-[2-[(1-oxo-2-propenyl)oxy]ethyl]poly(difluoromethylene)

CAS RN	459415-06-6
Chemical Name	2-Propenoic acid, 2-methyl-, 2-methylpropyl ester, polymer with butyl 2-propenoate and 2,5-furandione, .gamma.-.omega.-perfluoro-C8-14-alkyl esters, tert-Bu benzenecarboperoxoate-initiated

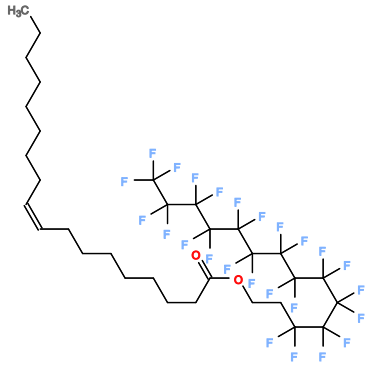
CAS RN	524729-93-9
Chemical Name	2-Propenoic acid, polymer with butyl 2-propenoate and 2,5-furandione, gamma-omega-perfluoro-C8-14-alkyl esters, potassium salts, tert-Bu benzenecarboperoxoate-initiated

CAS RN	500701-62-2
Chemical Name	2-Propenoic acid, 2-methyl-, 2-(diethylamino)ethyl ester, polymer with alpha-fluoro-omega-[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]poly(difluoromethylene), acetate (salt)

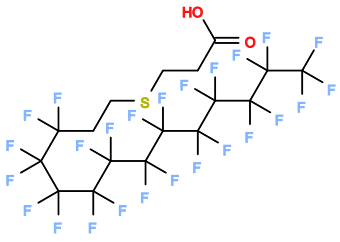
Carboxylic Acid and Ester Derivatives

CAS RN	125768-41-4
Chemical Name	9-Octadecenoic acid (9*Z*)-, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluorododecyl ester
Synonyms	10:2 fluorotelomer oleate
Structural Formula	
Molecular Formula	$C_{30}H_{37}F_{21}O_2$
Molecular Weight (g/mol)	828.58
SMILES	C(F)(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)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCOC(=O)CCCCCCC\C=C/CCCCCCCC

CAS RN	220237-52-5
Chemical Name	9-Octadecenoic acid (9*Z*)-, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecyl ester

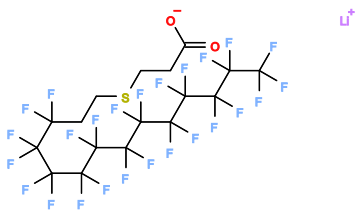
Synonyms	12:2 fluorotelomer oleate
Structural Formula	
Molecular Formula	$C_{32}H_{37}F_{25}O_2$
Molecular Weight (g/mol)	928.60
SMILES	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCOC(=O)CCCCCCC\C=C/CCCCCCCC

The substance represented by CAS RN 65530-83-8 is a mixture of homologous compounds with perfluorinated segments of various lengths. Representative chemical identity information is provided below.

CAS RN	65530-83-8
Chemical Name	Poly(difluoromethylene), .alpha.-[2-[(2-carboxyethyl)thio]ethyl]-.omega.-fluoro-
Synonyms	.alpha.-[2-[(2-carboxyethyl)thio]ethyl]-.omega.-fluoropoly(difluoromethylene)
Representative Structural Formula	
Representative	$C_{17}H_9F_{25}O_2S$

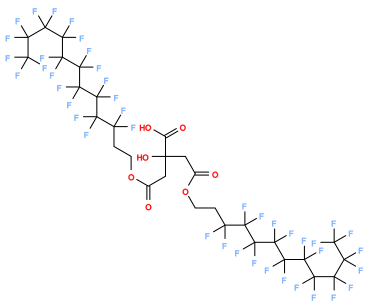
Molecular Formula	
Representative Molecular Weight (g/mol)	752.28
Representative SMILES	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCSCCC(=O)O

The substance represented by CAS RN 65530-69-0 is a mixture of homologous compounds with perfluorinated segments of various lengths. Representative chemical identity information is provided below.

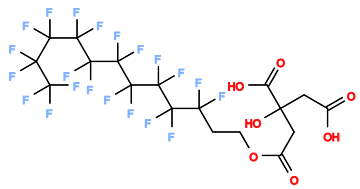
CAS RN	65530-69-0
Chemical Name	Poly(difluoromethylene), .alpha.-[2-[(2-carboxyethyl)thio]ethyl]-.omega.-fluoro-, lithium salt
Synonyms	lithium .alpha.-[2-[(2-carboxyethyl)thio]ethyl]-.omega.-fluoropoly(difluoromethylene)
Representative Structural Formula	
Representative Molecular Formula	$C_{17}H_8F_{25}LiO_2S$
Representative Molecular Weight (g/mol)	758.21
Representative SMILES	C(F)(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)C(F)(F)C(F)(F)CCSCCC(=O)[O-].[Li+]

CAS RN	65530-59-8
Chemical Name	Poly(difluoromethylene), .alpha.-fluoro-.omega.-(2-hydroxyethyl)-, 2-hydroxy-1,2,3-propanetricarboxylate (3:1)

The substance represented by CAS RN 65605-57-4 is a mixture of homologous compounds with perfluorinated segments of various lengths. Representative chemical identity information is provided below.

CAS RN	65605-57-4
Chemical Name	Poly(difluoromethylene), .alpha.-fluoro-.omega.-(2-hydroxyethyl)-, hydrogen 2-hydroxy-1,2,3-propanetricarboxylate
Synonyms	.alpha.-fluoro-.omega.-(2-hydroxyethyl)poly(difluoromethylene), hydrogen 2-hydroxy-1,2,3-propanetricarboxylate
Representative Structural Formula	
Representative Molecular Formula	$C_{30}H_{14}F_{42}O_7$
Representative Molecular Weight (g/mol)	1284.36
Representative SMILES	C(O)(CC(=O)OCCC(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)C(F)(F)(F))(CC(=O)OCCC(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)C(F)(F)(F))(C(=O)O)

The substance represented by CAS RN 65605-56-3 is a mixture of homologous compounds with perfluorinated segments of various lengths. Representative chemical identity information is provided below.

CAS RN	65605-56-3
Chemical Name	Poly(difluoromethylene), .alpha.-fluoro-.omega.-(2-hydroxyethyl)-, dihydrogen 2-hydroxy-1,2,3-propanetricarboxylate
Synonyms	.alpha.-fluoro-.omega.-(2-hydroxyethyl)poly(difluoromethylene), dihydrogen 2-hydroxy-1,2,3-propanetricarboxylate
Representative Structural Formula	
Representative Molecular Formula	$C_{18}H_{11}F_{21}O_7$
Representative Molecular Weight (g/mol)	738.24
Representative SMILES	C(O)(CC(=O)OCCC(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)C(F)(F)C(F)(F)(F))(CC(=O)O)(C(=O)O)

CAS RN	94095-37-1
Chemical Name	Pentanoic acid, 4,4-bis[(.gamma.-.omega.-perfluoro-C6-12-alkyl)thio] derivatives, compounds with diethanolamine

CAS RN	71608-61-2
Chemical Name	Pentanoic acid, 4,4-bis[(.gamma.-.omega.-perfluoro-C8-20-alkyl)thio] derivatives, compounds with diethanolamine

CAS RN	253682-98-3
Chemical Name	Butanedioic acid, monopolyisobutylene derivs., 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluorododecyl ester

CAS RN	253682-97-2
Chemical Name	Butanedioic acid, monopolyisobutylene derivs., 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluoro tetradecyl ester

Urethane Polymers

CAS RN	68891-05-4
Chemical Name	Ethene, tetrafluoro-, homopolymer, .alpha.-fluoro-.omega.-(2-hydroxyethyl)-, citrate, reaction products with 1,6-diisocyanatohexane

CAS RN	376364-33-9
Chemical Name	Alcohols, C8-14, gamma-omega-perfluoro, polymers with alpha-fluoro-omega-[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]poly(difluoromethylene), methanol, stearyl acrylate, stearyl methacrylate, 2,4-TDI and vinyl chloride

CAS RN	135228-60-3
Chemical Name	Hexane, 1,6-diisocyanato-, homopolymer, gamma-omega-perfluoro-C6-20-alc.-blocked

CAS RN	144468-32-6

Chemical Name	1,3-Propanediol, 2,2-bis(bromomethyl)-, reaction products with ethanethiol-tetrafluoroethylene telomer, polymers with 1,6-diisocyanato-2,2,4(or 2,4,4)-trimethylhexane, 2-heptyl-3,4-bis(9-isocyanatononyl)-1-pentylcyclohexane and 2,2'-(methylimino)bis[ethanol]

CAS RN	118102-37-7
Chemical Name	Alcohols, C8-14, .gamma.-.omega.-perfluoro, reaction products with epichlorohydrin, polyethylene glycol monomethyl ether and *N*,*N*',2-tris(6-isocyanatohexyl)imidodicarbonic diamide

CAS RN	118102-38-8
Chemical Name	Alcohols, C8-14, .gamma.-.omega.-perfluoro, reaction products with epichlorohydrin, tetrahydrofuran homopolymer and *N*,*N*',2-tris(6-isocyanatohexyl)imidodicarbonic diamide

CAS RN	332076-28-5
Chemical Name	2-Oxepanone, homopolymer, decyl perfluoro-C8-14-alkyl esters, reaction products with 1H-imidazole-1-propanamine, polyethylene-polypropylene glycol and TDI homopolymer

CAS RN	332076-33-2
Chemical Name	2-Oxepanone, homopolymer, decyl perfluoro-C8-14-alkyl esters, reaction products with 1H-imidazole-1-propanamine and TDI homopolymer

CAS RN	332076-34-3
Chemical Name	2-Oxepanone, homopolymer, decyl perfluoro-C8-14-alkyl esters, reaction products with 1H-imidazole-1-propanamine, polyethylene glycol and TDI homopolymer

CAS RN	68990-40-9
Chemical Name	Fatty acids, C18-unsaturated, dimers, diisocyanates, polymers with 2,3-bis(.gamma.-.omega.-perfluoro-C4-18-alkyl)-1,4-butanediol, 1,6-diisocyanato-2,2,4(or 2,4,4)-trimethylhexane and 2,2'-(methylimino)bis[ethanol]

CAS RN	253873-70-0
Chemical Name	Alcohols, C8-14, gamma-omega-perfluoro, polymers with 1,6-diisocyanatohexane, ethylene glycol, glycidol and 2,4-TDI

CAS RN	329201-80-1
Chemical Name	Imidodicarbonic diamide, *N*,*N*'2-tris(6-isocyanatohexyl)-, reaction products with ethylene glycol, alpha- fluoro-, omega-[2[(1-oxo- 2-propenyl)oxy]ethyl]poly(difluoromethylene), glycidol and 2,4-TDI

CAS RN	254889-72-0
Chemical Name	Imidodicarbonic diamide, *N*,*N*',2-tris(6-isocyanatohexyl)-, reaction products with 3-chloro-1,2-propanediol, ethylene, iodoethane and tetrafluoroethylene

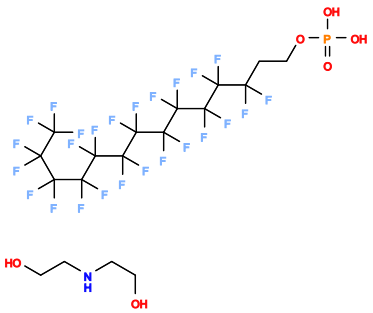
CAS RN	254889-79-7
Chemical Name	Methanol, reaction products with 1,6-diisocyanatohexane, ethylene, ethylene oxide, iodoethane and tetrafluoroethylene

CAS RN	428842-38-0
Chemical Name	Hexane, 1,6-diisocyanato-, homopolymer, alpha-fluoro-omega-(hydroxyethyl)poly(difluoromethylene)- and Me Et ketone oxime- and

polyethylene glycol mono-Me ether-blocked

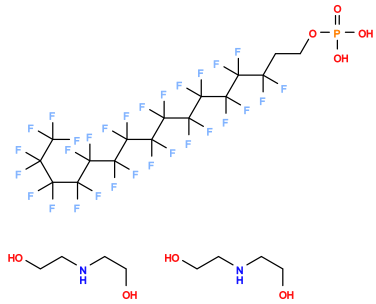
Phosphate Esters

The substance represented by CAS RN 65530-74-7 is a mixture of homologous compounds with perfluorinated segments of various lengths. Representative chemical identity information is provided below.

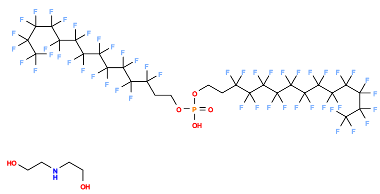
CAS RN	65530-74-7
Chemical Name	Ethanol, 2,2'-iminobis-, compd. with alpha-fluoro-omega-[2-(phosphonooxy)ethyl]poly(difluoromethylene) (1:1)
Representative Structural Formula	
Representative Molecular Formula	$C_{18}H_{17}F_{25}NO_6P$
Representative Molecular Weight (g/mol)	849.26
Representative SMILES	OCCNCCO.P(=O)(O)(O)(OCCC(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)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)C(F)(F)F)

The substance represented by CAS RN 65530-63-4 is a mixture of homologous compounds with perfluorinated segments of various lengths. Representative chemical identity information is provided below.

CAS RN	65530-63-4
Chemical Name	Ethanol, 2,2'-iminobis-, compd. with alpha-fluoro-omega-[2-(phosphonooxy)ethyl]poly(difluoromethylene) (2:1)

Representative Structural Formula	
Representative Molecular Formula	$C_{24}H_{27}F_{29}N_2O_8P$
Representative Molecular Weight (g/mol)	1054.42
Representative SMILES	OCCNCCO.OCCNCCO.P(O)(O)(=O)(OCCC(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)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)(F))

The substance represented by CAS RN 65530-64-5 is a mixture of homologous compounds with perfluorinated segments of various lengths. Representative chemical identity information is provided below.

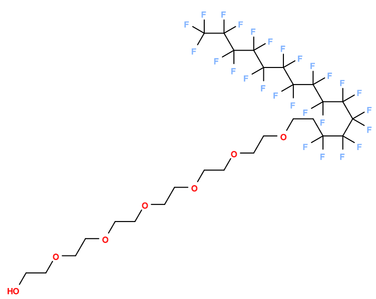
CAS RN	65530-64-5
Chemical Name	Ethanol, 2,2'-iminobis-, compd. with alpha,alpha'-[phosphinicobis(oxy-2,1-ethanediyl)]bis[omega-fluoropoly(difluoromethylene)] (1:1)
Representative Structural Formula	
Representative Molecular Formula	$C_{32}H_{20}F_{50}NO_6P$
Representative Molecular Weight	1495.40

(g/mol)	
Representative SMILES	OCCNCCO.P(O)(=O)(OCCC(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)C(F)(F)C(F)(F)C(F)(F)C(F)(F)(F))(OCCC(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)C(F)(F)C(F)(F)C(F)(F)C(F)(F)(F))

CAS RN	74499-44-8
Chemical Name	Phosphoric acid, gamma-omega-perfluoro-C8-16-alkyl esters, compds. with diethanolamine

Polyglycol Derivatives

The substance represented by CAS RN 65545-80-4 is a UVCB. This substance has perfluorinated segments and poly(ethylene glycol) chains of various lengths. Representative chemical identity information is provided below.

CAS RN	65545-80-4
Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-hydro-.omega.-hydroxy-, ether with .alpha.-fluoro-.omega.-(2-hydroxyethyl)poly(difluoromethylene) (1:1)
Representative Structural Formula	
Representative Molecular Formula	$C_{27}H_{29}F_{27}O_7$
Representative Molecular Weight (g/mol)	978.47

Representative SMILES	C(F)(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)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCOCCOCCOCCOCCOCCOCCO

CAS RN	70983-59-4
Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-methyl-.omega.-hydroxy-, 2-hydroxy-3-[(.gamma.-.omega.-perfluoro-C6-20-alkyl)thio]propyl ethers

Alkyl Ammonium and Amine Derivatives

CAS RN	98219-29-5
Chemical Name	Betaines, *N*-(hydroxyethyl)-*N*-methyl-*N*-(2-sulfoethyl)-*N*-(1,1,2-trihydroperfluoro-C8-14-2-alkenyl)

CAS RN	115340-82-4
Chemical Name	Betaines, (hydroxyethyl)methyl(.gamma.,.omega.-perfluoro-C8-14-.beta.-alkenyl)(2-sulfopropyl)

CAS RN	92129-34-5
Chemical Name	Quaternary ammonium compounds, (hydroxyethyl)dimethyl(.gamma.-.omega.-perfluoro-C8-14-.beta.-alkenyl), methyl sulfates

CAS RN	115535-36-9
Chemical Name	Quaternary ammonium compounds, trimethyl(.delta.-.omega.-perfluoro-C8-14-.beta.-alkenyl), chlorides

CAS RN	127133-57-7
Chemical Name	Quaternary ammonium compounds, diethylmethyl(.gamma.-.omega.-perfluoro-C8-14-.beta.-alkenyl), methyl sulfates

CAS RN	145477-02-7
Chemical Name	Quaternary ammonium compounds, diethyl methyl (.gamma.-.omega.-perfluoro-C8-14-.beta.-alkenyl), tetraphenyl borates

CAS RN	153325-45-2
Chemical Name	Quaternary ammonium compounds, diethyl methyl (.gamma.-.omega.-perfluoro-C8-14-.beta.-alkenyl), tetrafluoroborates

CAS RN	65530-57-6
Chemical Name	Poly(difluoromethylene), .alpha.-fluoro-.omega.-[2-[[2-(trimethylammonio)ethyl]thio]ethyl]-, methyl sulfate

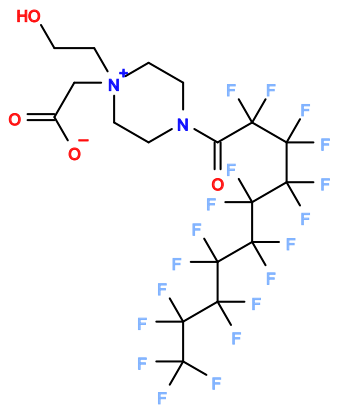
CAS RN	71002-41-0
Chemical Name	Poly(difluoromethylene), .alpha.-[2-(acetyloxy)-2-[(carboxymethyl)dimethylammonio]ethyl]-.omega.-fluoro-, hydroxide, inner salt

CAS RN	68187-47-3
Chemical Name	1-Propanesulfonic acid, 2-methyl-, 2-[[1-oxo-3-[(.gamma.,.omega.-perfluoro-C4-16-alkyl)thio]propyl]amino] derivatives, sodium salts

CAS RN	68187-25-7
Chemical Name	Butanoic acid, 4-[[3-(dimethylamino)propyl]amino]-4-oxo-, 2(or 3)-[(.gamma.-.omega.-perfluoro-C6-20-alkyl)thio] derivatives

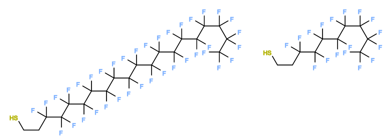
CAS RN	70983-60-7
Chemical Name	1-Propanaminium, 2-hydroxy-*N*,*N*,*N*-trimethyl-, 3-[(gamma-omega-perfluoro-C6-20-alkyl)thio] derivs., chlorides

Miscellaneous Derivatives

CAS RN	71356-38-2
Chemical Name	Piperazinium, 1-(carboxymethyl)-1-(2-hydroxyethyl)-4-(2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-nonadecafluoro-1-oxodecyl)-, hydroxide, inner salt
Synonyms	1-(2-hydroxyethyl)-4-(perfluorooxodecyl)piperazinium
Structural Formula	
Molecular Formula	$C_{18}H_{15}F_{19}N_2O_4$
Molecular Weight	684.29

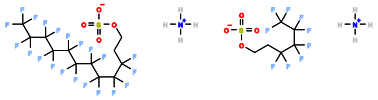
SMILES	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(=O)N1CC[N+](CC(=O)[O-])(CCO)CC1

The substance represented by CAS RN 68140-21-6 is a UVCB. Representative chemical identity information is provided for the two end members of this substance below. This substance is a mixture of fluorotelomer thiols with chains of eight to eighteen perfluorinated carbons.

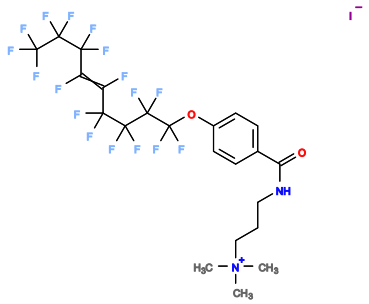
CAS RN	68140-21-6
Chemical Name	Thiols, C10-20, .gamma.-.omega.-perfluoro
Representative Structural Formula	
Representative Molecular Formula	$C_{10}H_5F_{17}S$ $C_{20}H_5F_{37}S$
Representative Molecular Weight (g/mol)	480.18 980.26
Representative SMILES	SCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)(F) SCCC(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)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)

The substance represented by CAS RN 68516-17-6 is a UVCB. Representative chemical identity information is provided for the two end members of this substance below. This substance contains a mixture of fluorotelomer sulfates with chains of four to ten perfluorinated carbons.

CAS RN	68516-17-6
Chemical Name	Sulfuric acid, mono(.gamma.-.omega.-perfluoro-C6-12-alkyl) esters, ammonium salts

Representative Structural Formula	
Representative Molecular Formula	$C_6H_8F_9NO_4S$ $C_{12}H_8F_{21}NO_4S$
Representative Molecular Weight (g/mol)	361.18 661.23
Representative SMILES	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)CCOS(=O)(=O)[O-].[NH4+] C(F)(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)C(F)(F)C(F)(F)CCOS(=O)(=O)[O-].[NH4+]

The substance represented by CAS RN 59493-72-0 has a perfluorinated nonenyl moiety and as such is not a precursor to perfluorononanoic acid (PFNA). This substance is a potential precursor to isomers of perfluorononenoic acid which are considered to be analogous to PFNA as outlined in the Environmental Fate section. As the location of the double bond in the nonenyl unit is not specified, the structure given below is representative only:

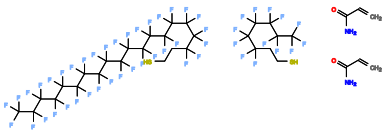
CAS RN	59493-72-0
Chemical Name	1-Propanaminium, 3-[[4-[(heptadecafluorononenyl)oxy]benzoyl]amino]-*N*,*N*,*N*-trimethyl-, iodide
Representative Structural Formula	
Molecular Formula	$C_{22}H_{20}F_{17}IN_2O_2$
Molecular Weight (g/mol)	794.28

SMILES	[N+](C)(C)(C)CCCNC(=O)c1ccc(OC((F)(F))C((F)(F))C((F)(F))C((F)(F))C(F)=C(F)C((F)(F))C((F)(F))C((F)(F)(F)))cc1.[I-]

CAS RN	84238-62-0
Chemical Name	Sulfuric acid, mono(.gamma.-.omega.-perfluoro-C8-12-alkyl) esters, ammonium salts

Other Polymers and Telomers

The substance represented by CAS RN 70969-47-0 is a UVCB. Representative chemical identity information is provided for component monomers. This substance contains a mixture of telomers with chains of six to eighteen perfluorinated carbons.

CAS RN	70969-47-0
Chemical Name	Thiols, C8-20, .gamma.-.omega.-perfluoro, telomers with acrylamide
Representative Structural Formula	
Representative SMILES	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCS.C(F)(F)(F)CCS C=CC(=O)N.C=CC(=O)N

CAS RN	113089-67-1
Chemical Name	Thiols, C4-20, .gamma.-.omega.-perfluoro, reaction products with methylated formaldehyde-1,3,5-triazine-2,4,6-triamine polymer

CAS RN	185630-70-0

Chemical Name	Alcohols, C8-14, .gamma.-.omega.-perfluoro, reaction products with epichlorohydrin and propylene oxide, trimethylamine-quaternized
CAS RN	65530-58-7
Chemical Name	Poly(difluoromethylene), .alpha.-fluoro-.omega.-(2-hydroxyethyl)-, ester with 2,15-bis(carboxymethyl)-4,13-dioxo-3,14-dioxa-5,12-diazahexadecane-1,2,15,16-tetracarboxylic acid (6:1)

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 and UVCBs. Based on the available data, most chemicals in this group are expected to be solids under ambient conditions (NICNAS, 2015c, d). The higher molecular weight chemicals, including the telomers and polymers, are expected to be involatile. However, the relatively lower molecular weight neutral organic substances may have some volatility. For example, data available for the analogue chemical, 8:2 FTOH (CAS RN 678-39-7), show that the vapour pressure values for this white waxy solid can be as high as 254 Pa at 25°C (NICNAS, 2015c, d).

Import, Manufacture and Use

Australia

In July 2006, NICNAS collected information on manufacture, importation and uses of perfluorinated chemicals including PFCA-related substances and products/mixtures containing these substances for the calendar years 2004 and 2005.

Information obtained by NICNAS indicated that:

- Two PFCA precursors were imported into Australia in 2005. One was a perfluorinated furan compound (0.25 kilograms) used as an analytical reagent. The other substance was a polymer containing a perfluoroalkylethyl ester moiety imported at 150 kilograms in 2005, which was used to formulate coatings for wood boards of internal wall cladding.
- Eight products containing PFCA precursors were imported into Australia during 2004 and 2005. Five of them were water/oil repellent products used for textiles, carpets, and masonry/cement surfaces. The remaining three products were used for automotive painting, glass treatment and ink cartridges. These eight PFCA precursors included five perfluoroalkylethyl chemicals/polymers and three fluorinated acrylate polymers. The total volume of the eight products was up to 33 300 kilograms per annum, with the majority of this being polymeric substances.

However, this information could be incomplete because the call for information did not specifically include the PFCA group (NICNAS, 2013).

Three of the chemicals in this group (CAS RNs 500701-62-2, 428842-38-0, and 59493-72-0) have previously been assessed as new chemicals under NICNAS, and they were subsequently added to the Inventory. The first two of these chemicals are discontinued products, and are no longer expected to be in active use.

It is noted that the chemicals in this group may be present in the environment due to historic use, breakdown of chemicals not included in this assessment, or release from pre-treated articles imported into Australia. However, release from these uses is beyond the scope of this assessment.

International

The neutral organic fluorotelomer derivatives in this group are used as industrial intermediates (ECHA, 2019a, OECD, 2011). Five of these chemicals (including 10:2 FTOH, 12:2 FTOH and 12:2 FTMAC) have recently been reported as in use in various Nordic countries (Nordic Council of Ministers, 2015). The two neutral organic UVCB substances (CAS RNs 68391-08-2 and 85631-54-5) are currently registered for use in the European Union, as is the polymer represented by CAS RN 101896-32-6 (ECHA, 2019a). In the United States of America (USA), the UVCB fluorotelomer alcohol (CAS RN 68391-08-2) is also reported to have been used in the recent past (US EPA, 2015).

An additional 20 chemicals in this group have also recently been reported to be in use in various Nordic countries. A number of polymers have use in a range of applications, including use in coating products, fabric protectors, textile impregnation agents, firefighting foam and carpet protectors. Similarly, the alkyl ammonium and amine derivatives (CAS RNs 68187-47-3 and 70983-60-7) appear to have use in fire-fighting foam, while the thio ethyl carboxylic acid and its lithium salt (CAS RNs 65530-83-8 and 65530-69-0) are reported to be used in cleaning products, polishing agents and products for motor vehicle repair. Three of the four phosphate esters in this group (CAS RNs 65530-64-5, 65530-74-7 and 65530-63-4), and one of the polyethylene glycol compounds (CAS RN 65545-80-4), are reported to be used in paints, lacquers and varnishes (Nordic Council of Ministers, 2015).

Conversely, a number of chemicals in this group appear to have limited use internationally. Twenty-five chemicals in this group (including 22 polymers) were not identified as being listed on the chemical inventories of any other country.

Data for one neutral organic derivative (CAS RN 85631-54-5) indicate that it is being used at between 100 and 1000 tonnes per annum in the European Union (ECHA, 2019a). No further volume data were identified for the chemicals in this group. Nevertheless, it is noted that it has previously been estimated that approximately 1000 tonnes of PFOA-related substances for textile and leather treatment are introduced per annum in the European Union, with a further 1000 to 10 000 tonnes imported in textile articles (ECHA, 2014).

Environmental Regulatory Status

Australia

A factsheet published by NICNAS recommends that industry seek alternatives to PFOA and chemicals that may degrade to PFOA, and ultimately aim to phase out use of these substances (NICNAS, 2013).

Some state governments in Australia have introduced regulations regarding the management of PFAScontaining 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). Firefighting foams that contain PFOA, PFOA precursor compounds or their higher homologues, where the total organic fluorine content equivalent to PFOA and higher homologues exceeds 50 mg/kg in foam concentrate must be withdrawn from service as soon as practicable.

Under the terms of the Inventory listings for CAS RNs 500701-62-2, 428842-38-0, and 59493-72-0, secondary notification conditions apply for introducers of these chemicals.

United Nations

Some of the discrete chemical constituents of a number of the substances in this group can degrade into PFOA according to the recent listing of PFOA, its salts and PFOA-related compounds on Annex A (Elimination) of the Stockholm Convention on Persistent Organic Pollutants (UNEP, 2001; 2019). The listing prohibits production and use of these chemicals for purposes other

than specific time-limited exemptions for specialised uses in the manufacture of semiconductors, photographic films, and certain textiles for use in the protection of workers from exposure to dangerous liquids. Australia has not yet ratified this amendment.

The chemicals in this group are not currently identified as ozone depleting substances (UNEP, 1987), or hazardous substances for the purpose of international trade (UNEP & FAO, 1998).

OECD

The chemicals in this group have not been sponsored for assessment under the Cooperative Chemicals Assessment Programme (CoCAP) (OECD, 2013).

The OECD has been leading an international collaboration on the scientific assessment of, and surveys of, perfluorinated chemicals. Since July 2000, Australia has been actively involved in this work through NICNAS.

Canada

Substances with a perfluorinated moiety of seven to twenty perfluorinated carbons directly bonded to any chemical moiety other than a fluorine, chlorine or bromine atom are listed under Schedule 1 (the Toxic Substances List) of the *Canadian Environmental Protection Act 1999* (CEPA) (Government of Canada, 2018c), which prohibits their manufacture, import, use or sale. Exemptions for certain uses of these chemicals where developments are underway or where there are currently no known alternatives are currently in force, but a proposal to further restrict the manufacture, import, use or sale of these chemicals has been released and is expected to be finalised by winter 2020 (Government of Canada, 2018a, b).

Twenty nine of the chemicals in this group are listed on the Canadian Domestic Substances List (DSL) (Government of Canada, 2019). Of these, 8 met the criteria under subsection 73(1) of CEPA during the Categorization of the DSL to be or potentially be PBT chemicals.

European Union

Four chemicals in this group (CAS RNs 85631-54-5, 68391-08-2, 101896-32-6, and 59493-72-0) are registered for use in the European Union under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation (ECHA, 2019a).

An additional 18 chemicals have been pre-registered, but not undergone the full registration process, under the REACH legislation (ECHA, 2019b).

United States of America

In January 2006, the United States Environmental Protection Agency (US EPA) launched a global PFOA stewardship program. The eight major companies that manufacture fluoropolymers and fluorotelomers committed to reduce facility emissions of all PFOA, PFOA precursors and related chemicals by 95% by no later than 2015 (compared to 2000 baseline) (US EPA, 2009).

Many of the chemicals in this group (39 substances) are listed on the inventory of chemicals manufactured or processed in the USA, as published under the *Toxic Substances Control Act 1976* (TSCA) (US EPA, 2018). The United States Environmental Protection Agency (US EPA) proposed a new Significant New Activity Rule for these chemicals in January 2015. Under the Rule, approval must be sought for new uses of these chemicals, including import in articles. The US EPA understands that existing uses of these chemicals will be phased out by December 2015 under a voluntary stewardship programme (US EPA, 2015).

The 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 data, a number of chemicals in this group may have use in a wide range of applications in Australia. Release to the environment may occur during the use and disposal of these chemicals, including the use and disposal of products containing the chemicals, and that of articles treated with commercial and domestic surface treatment products. Use in firefighting foams is expected to have the potential for significant environmental emissions depending on the location of release, and the containment measures in place.

The environmental degradants of primary concern for the chemicals in this group are long-chain perfluorinated carboxylic acids. These chemicals are purely of anthropogenic origin. Perfluorooctanoic acid, which has previously been assessed by NICNAS, has been identified as a PBT substance (NICNAS, 2015a). The longer chain perfluorocarboxylic acids are also expected to have similar environmental concerns (ECHA, 2012a, b, c, d , Environment Canada, 2012, NITE, 2014, US EPA, 2009).

Most chemicals in this group contain a perfluorinated chain linked to another functional group or polymer chain through an ethylene unit. Based on a number of studies that have demonstrated potential for 8:2 fluorotelomer derivatives to degrade through abiotic or biotic mechanisms to 8:2 FTOH (NICNAS, 2015c), these chemicals are assumed to have potential to similarly degrade to their respective fluorotelomer ethyl alcohol. Environmental fate data available for 8:2 FTOH indicate that subsequent biotransformation of the fluorotelomer ethyl alcohol will yield a perfluorinated carboxylic acid with one less perfluorinated carbon (Butt, et al., 2014, De Voogt, 2010, Dinglasan, et al., 2004). The potential environmental degradation pathway for the other chemicals in this group has been less studied. Nevertheless, previous work has suggested that these chemicals may also degrade to perfluorocarboxylic acids (OECD, 2007).

Monitoring data have identified a range of FTOH and perfluorinated carboxylic acids in the environment. Various studies have identified 4:2 FTOH, 6:2 FTOH, 8:2 FTOH, 10:2 FTOH and 12:2 FTOH in air samples globally at concentrations up to 275 picograms per cubic metre (Barber, et al., 2007, Jahnke, et al., 2007, NICNAS, 2015c, d, Stock, et al., 2004). In addition, a range of perfluorocarboxylic acids (from perfluorohexanoic acid through to perfluorotridecanoic acid) have been detected in Australian water and/or sediment samples from the Parramatta and Brisbane river catchments. Concentrations in water samples ranged from 0.04 to 11 nanograms per litre, while concentrations in sediment were generally below 1 nanogram per gram (Gallen, et al., 2014, Thompson, et al., 2011).

It is noted that there are multiple potential sources of long-chain FTOHs and perfluorocarboxylic acids in the environment including past industrial use of other fluorinated chemicals contaminated with these substances, use in articles, or from the use of other fluorinated chemicals which degrade to these substances in the environment.

The environmental fate of substances with long perfluorinated alkene chains is currently unknown. This is a gap in the available environmental hazard data for highly fluorinated organic chemicals. Hence, it is assumed that substances such as the one represented by CAS RN 59493-72-0 will degrade to perfluorinated alkenoic acids, and that they will have similar mobility and persistence in the environment as perfluorinated alkanoic acids with the same carbon atom chain length. NICNAS may reconsider these assumptions if relevant and reliable studies of the environmental fate of substances with long perfluorinated alkene chains are made available.

Environmental Effects

Currently available ecotoxicity data for PFOA and its shorter perfluorocarboxylic acid homologues are summarised in the IMAP Environment Tier II assessment for Perfluorooctanoic Acid (PFOA) and its Direct Precursors, the IMAP Environment Tier II assessment for Perfluoroheptanoic Acid (PFHpA) and its Direct Precursors, and the IMAP Environment Tier II assessment for Short-Chain Perfluorocarboxylic Acids and their Direct Precursors. Information currently available indicates that the short-chain perfluorocarboxylic acids have low ecotoxicity, while PFOA has been found to cause chronic, intergenerational toxicity at low concentrations (0.1 mg/L) in fish (NICNAS, 2015a, b).

Limited ecotoxicity data are available for the longer chain perfluorocarboxylic acids. Data available for perfluorononanoic acid (PFNA) indicate low acute toxicity to algae (median effective concentration values > 100 mg/L) (Latala, et al., 2009). No chronic toxicity data were identified for these chemicals. However, multiple studies have demonstrated that toxicity of perfluorocarboxylic acids increases with perfluorinated chain length (Barmentlo, et al., 2015, Latala, et al., 2009). Therefore, the longer chain perfluorocarboxylic acids are expected to have no lower chronic toxicity than PFOA.

The parent 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 long-chain perfluorinated carboxylic acids into the environment.

Categorisation of Environmental Hazard

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

It is noted that direct precursors to PFOA are categorised as persistent, bioaccumulative and toxic (PBT) substances according to domestic environmental hazard criteria (NICNAS, 2015a). In addition, data available for the longer-chain perfluorocarboxylic acids demonstrate significant persistence and bioaccumulation potential (ECHA, 2012a, b, c , d, NITE, 2014, US EPA, 2009). Some data also indicate potential for high chronic toxicity (Barmentlo, et al., 2015, Latala, et al., 2009 , US EPA, 2009).

Risk Characterisation

The chemicals in this group may degrade to long-chain perfluorocarboxylic acids, which are expected to have PBT hazard characteristics. 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.

Due to their persistence, PBT chemicals have the potential to become widely dispersed environmental contaminants. Once in the environment, persistent chemicals that are also highly bioaccumulative pose an increased risk of accumulating in exposed organisms and of causing adverse effects. They may also biomagnify through the food chain resulting in very high internal concentrations, especially in top predators. Importantly, it is difficult or impossible to reverse the adverse effects of PBT chemicals once they have been released to the environment.

Key Findings

Based on international data, some of the chemicals in this group may have current industrial use in a wide range of applications in Australia, including various surface treatment products, firefighting foams and paints.

Available data indicate that chemicals in this group have the potential to degrade to long-chain perfluorocarboxylic acids. Therefore, the principal risk posed by the chemicals in this group if emitted to the environment is assumed to result from cumulative releases of these degradation products. The C_8 perfluorocarboxylic acid, PFOA, has previously been identified as a PBT chemical and is therefore of high concern to the environment. Available data indicate that the longer chain homologues of PFOA will have similar PBT hazard characteristics and they consequently pose a similar level of concern.

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 in this assessment to characterise these potential hazards for each individual chemical.

It is noted that significant volumes of the chemicals in this group may also be imported into Australia as components of finished articles. However, release from these articles and the associated environmental risks are beyond the scope of this assessment.

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 Perfluorocarboxylic Acids (PFCA) (NICNAS, 2015e).

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 (AICS), and are available to be introduced into Australia without the requirement for 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 PFOA have been classified as Chronic Aquatic Category 1 (H410: Very toxic to aquatic life with long lasting effects) under the GHS (NICNAS, 2015a).

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