Indirect precursors to short-chain perfluorocarboxylic acids: Environment tier II assessment

12 December 2019

CAS Registry Numbers: 647-42-7, 2144-53-8, 1799-84-4, 432-08-6, 338-84-1, 311-89-7, 54950-05-9, 253682-99-4, 220237-47-8, 38436-16-7, 163702-07-6, 355-80-6, 72494-14-5, 83003-52-5, 97331-50-5

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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

Acronyms & Abbreviations

Grouping Rationale

This Tier II assessment considers the environmental risks associated with the industrial uses of 12 per and polyfluoroalkyl substances (PFASs) which are all indirect precursors to short-chain perfluorocarboxylic acids (perfluoroalkyl carboxylic acids; PFCAs). The assessment also includes a small group of four fluorinated organic chemicals which may degrade to polyfluorinated organic acids that are similar to short-chain PFCAs.

The PFASs considered in this assessment include important fluorotelomer and fluorotelomer methacrylate industrial intermediates. These chemicals are used in the manufacture of polymers with perfluorinated side-chains, and they were introduced by industry as alternatives to other chemicals which may degrade into long-chain perfluoroalkyl acids (Buck, et al., 2011). All of the PFASs in this group are expected to degrade in the environment into one or more of the short-chain PFCAs including perfluorohexanoic acid (PFHxA), perfluoropentanoic acid (PFPeA), and perfluorobutanoic acid (PFBA).

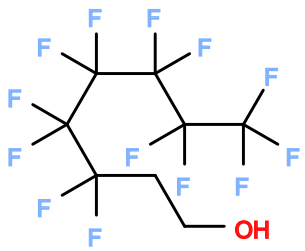
Perfluoroalkyl carboxylic acids are of concern globally due to their extreme persistence in the environment. The long-chain perfluoroalkyl acid, perfluorooctanoic acid (PFOA), and its ammonium salt, have been categorised as persistent, bioaccumulative and toxic (PBT) substances according to domestic environmental hazard criteria (NICNAS, 2015a, b). Chemicals with these hazard characteristics are of high concern to the environment and PFOA (and substances which may

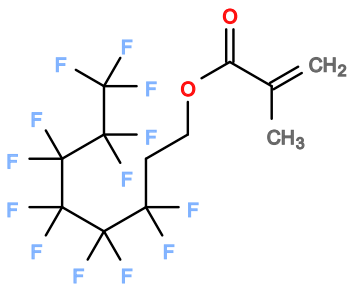
degrade to PFOA) are subject to increasingly stringent regulatory controls in other developed countries (NICNAS, 2015a, b). However, the short-chain PFCAs have been assessed as being of lower overall concern to the environment based on the available information (NICNAS, 2015c).

NICNAS has developed an action plan to assess and manage chemicals with a perfluorinated chain of four or more carbons which may degrade to perfluorocarboxylic acids, perfluoroalkyl sulfonates and similar chemicals (NICNAS, 2018a). 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. Data for other perfluorinated chemicals suggest that the major product of environmental biodegradation will be perfluorocarboxylic acids with one less perfluorinated carbon atom (NICNAS, 2018a).

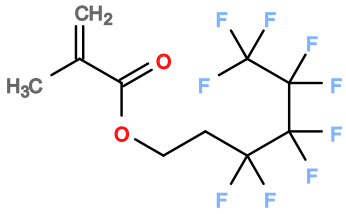
The degradation of PFHxA, PFPeA and PFBA is very slow compared with their rate of formation from degradation of the precursors. Therefore, the amount of PFHxA, PFPeA and PFBA in the environment (general or local) is expected to be higher than that of any of the precursors. Therefore, it will be assumed for the purposes of this assessment that the primary risk posed by the PFASs in this group results from release of PFHxA, PFPeA and PFBA to the environment. The IMAP Environment Tier II Assessment for Short-Chain Perfluorocarboxylic Acids and their Direct Precursors (NICNAS, 2015c) has been used as a reference assessment.

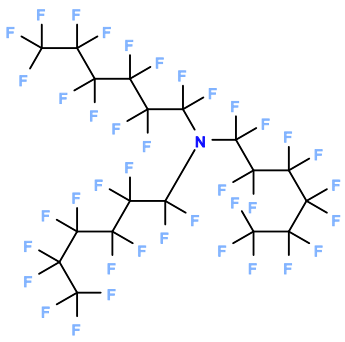
Chemical Identity

CAS RN	647-42-7
Chemical Name	1-Octanol, 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoro-
Synonyms	6:2 FTOH 6:2 fluorotelomer alcohol
Structural Formula	
Molecular Formula	$C_8H_5F_{13}O$
Molecular Weight (g/mol)	364.10
SMILES	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCO

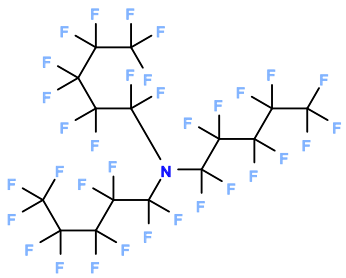
CAS RN	2144-53-8
Chemical Name	2-Propenoic acid, 2-methyl-, 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl ester
Synonyms	6:2 FTMAC 6:2 fluorotelomer methacrylate
Structural Formula	
Molecular Formula	$C_{12}H_9F_{13}O_2$
Molecular Weight (g/mol)	432.18
SMILES	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCOC(=O)C(=C)C

CAS RN	1799-84-4
Chemical Name	2-Propenoic acid, 2-methyl-, 3,3,4,4,5,5,6,6,6-nonafluorohexyl ester
Synonyms	4:2 FTMAC 4:2 fluorotelomer methacrylate
Structural Formula	

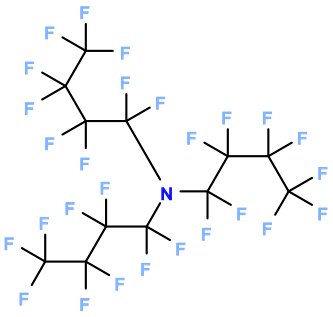
	
Molecular Formula	$C_{10}H_9F_9O_2$
Molecular Weight (g/mol)	332.16
SMILES	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)CCOC(=O)C(=C)C

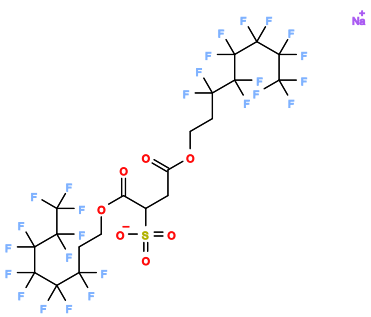
CAS RN	432-08-6
Chemical Name	1-Hexanamine, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-*N*,*N*-bis(tridecafluorohexyl)-
Synonyms	perfluorotrihexylamine
Structural Formula	
Molecular Formula	$C_{18}F_{39}N$
Molecular Weight (g/mol)	971.14

SMILES	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)N(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F

CAS RN	338-84-1
Chemical Name	1-Pentanamine, 1,1,2,2,3,3,4,4,5,5,5-undecafluoro-*N*,*N*-bis(undecafluoropentyl)-
Synonyms	perfluorotripentylamine
Structural Formula	
Molecular Formula	$C_{15}F_{33}N$
Molecular Weight (g/mol)	821.11
SMILES	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)N(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F

CAS RN	311-89-7
Chemical Name	1-Butanamine, 1,1,2,2,3,3,4,4,4-nonafluoro-*N*,*N*-bis(nonafluorobutyl)-
Synonyms	perfluorotributylamine

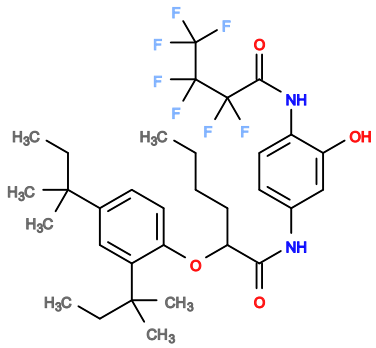
Structural Formula	
Molecular Formula	$C_{12}F_{27}N$
Molecular Weight (g/mol)	671.09
SMILES	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)N(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F

CAS RN	54950-05-9
Chemical Name	Butanedioic acid, sulfo-, 1,4-bis(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl) ester, sodium salt
Synonyms	sodium 1,4-bis(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl) sulphonatosuccinate
Structural Formula	
Molecular Formula	$C_{20}H_{11}F_{26}NaO_7S$

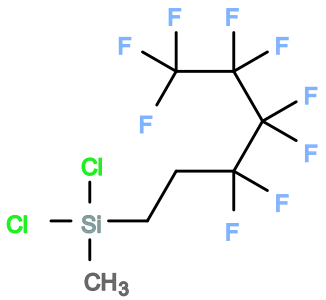
Molecular Weight (g/mol)	912.31
SMILES	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCOC(=O)C(CC(=O)OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)[O-].[Na+]

CAS RN	253682-99-4
Chemical Name	Butanedioic acid, monopolyisobutylene derivs., 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl ester

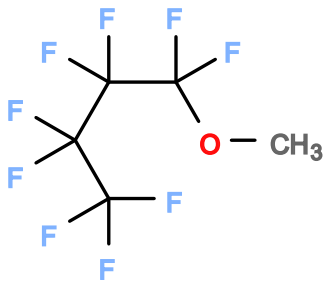
CAS RN	220237-47-8
Chemical Name	9-Octadecenoic (*Z*-)-, reaction products with 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoro-1-octanol

CAS RN	2923-93-5
Chemical Name	Hexanamide, 2-[2,4-bis(1,1-dimethylpropyl)phenoxy]-*N*-[4-[(2,2,3,3,4,4,4-heptafluoro-1-oxobutyl)amino]-3-hydroxyphenyl]-
Structural Formula	
Molecular Formula	$C_{32}H_{41}F_7N_2O_4$

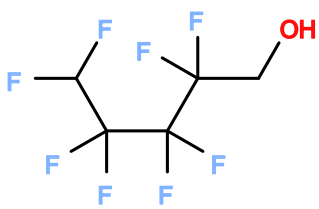
Molecular Weight (g/mol)	650.67
SMILES	c1c(OC(C(=O)Nc2ccc(NC(=O)C(F)(F)C(F)(F)C(F)(F)(F))c(O)c2)CCCC)c(C(C)(C)CC)cc(C(C)(C)CC)c1

CAS RN	38436-16-7
Chemical Name	Silane, dichloromethyl(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-
Synonyms	1*H*,1*H*,2*H*,2*H*-perfluorohexylmethyldichlorosilane
Structural Formula	
Molecular Formula	$C_7H_7Cl_2F_9Si$
Molecular Weight (g/mol)	361.11
SMILES	C[Si](CCC(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(Cl)Cl

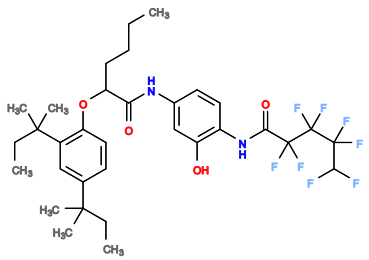
CAS RN	163702-07-6
Chemical Name	1-Methoxy 1,1,2,2,3,3,4,4,4-nonafluorobutane
Synonyms	methoxyperfluorobutane

Structural Formula	
Molecular Formula	$C_5H_3F_9O$
Molecular Weight (g/mol)	250.06
SMILES	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)OC

The following four chemicals have been grouped together because they all have a fully fluorinated carbon atom chain segment terminated by a difluoromethyl group. Although they lack the terminal perfluoromethyl group that is common to the better characterised PFASs, the highly fluorinated alkyl chains in each of these substances are expected to be resistant to typical biodegradation process. All four chemicals are potential precursors to recalcitrant polyfluorinated carboxylic acids that are analogous to short-chain PFCAs as outlined in the Environmental Exposure section.

CAS RN	355-80-6
Chemical Name	1-Pentanol, 2,2,3,3,4,4,5,5-octafluoro-
Synonyms	2,2,3,3,4,4,5,5-octafluoro-1-pentanol 1*H*,1*H*,5*H*-octafluoro-1-pentanol
Structural Formula	
Molecular Formula	$C_5H_4F_8O$

Molecular Weight (g/mol)	232.07
SMILES	C(F)(F)(C(F)(F)C(F)(F)C(F)F)CO

CAS RN	72494-14-5
Chemical Name	Hexanamide, 2-[2,4-bis(1,1-dimethylpropyl)phenoxy]-*N*-[3-hydroxy-4-[(2,2,3,3,4,4,5,5-octafluoro-1-oxopentyl)amino]phenyl]-
Structural Formula	
Molecular Formula	$C_{33}H_{42}F_8N_2O_4$
Molecular Weight (g/mol)	682.70
SMILES	CCCCC(C(=O)NC1=CC(=C(C=C1)NC(=O)C(C(C(C(F)F)(F)F)(F)F)(F)F)O)OC2=C(C=C(C=C2)C(C)(C)CC)C(C)(C)CC

CAS RN	83003-52-5
Chemical Name	Hexanamide, 2-[2,4-bis(1,1-dimethylpropyl)phenoxy]-*N*-[3-hydroxy-4-[(octafluoro-1-oxopentyl)amino]phenyl]-

CAS RN	97331-50-5

Chemical Name	Hexanamide, 6-[2,4-bis(1,1-dimethylpropyl)phenoxy]-*N*-[3-hydroxy-4-[(octafluoro-1-oxopentyl)amino]phenyl]-

Physical and Chemical Properties

Available physical and chemical property data for three members of the group are presented below (ENVIRON, 2014; NICNAS, 2006; TOXNET, 2003):

Chemical	perfluorotributylamine	6:2 FTOH	methoxyperfluorobutane
Physical Form	liquid	liquid	liquid
Melting Point	-50°C (exp.)	Not available	< -25°C (exp.)
Boiling Point	178°C (exp.)	Not available	60.5-62°C (exp.)
Vapour Pressure	73.6 Pa (exp.)	18-44 Pa (exp.)	27 700 Pa (exp.)
Water Solubility	not available	18.8 mg/L (exp.)	8.47 mg/L (exp.)

All three chemicals are volatile or highly volatile liquids under ambient conditions.

The reported vapour pressure values for 6:2 FTOH are between 18 and 44 Pa at 25°C (ENVIRON, 2014). However, the measured vapour pressure can be dependent on the method employed. For example, some measurements and extrapolations provide a vapour pressure as high as 876 Pa for this chemical (Lei, et al., 2004). The reported water solubility value for 6:2 FTOH indicates that this chemical has moderate solubility in water.

The methacrylate monomer, 6:2 FTMAC, is only slightly soluble in water (0.378 mg/L) and is volatile (8.6 Pa at 25°C) (ENVIRON, 2014). Based on these characteristics, 6:2 FTMAC is expected to be highly volatile from water (calculated Henry's law constant = 9833 Pa m^3/mole). The homologous methacrylate, 4:2 FTMAC, is also expected to be highly volatile from water.

The polyfluoroalkyl silane, 1*H*,1*H*,2*H*,2*H*-perfluorohexylmethyldichlorosilane (CAS RN 38436-16-7), is expected to hydrolyse rapidly in water and release polyfluoroalkylsilanols that may undergo condensation reactions to form fluoro-organic polysiloxanes (NICNAS, 2018b; REACH, 2019).

No reliable experimental physical and chemical property data were located for the other members of this group. The chemicals in this group will have a range of physical and chemical properties given the differences in chemical structure.

Import, Manufacture and Use

Australia

Methoxyperfluorobutane is used as a cleaning and heat transfer agent, and as a cosmetic ingredient. The chemical is not manufactured or formulated in Australia. It is imported in formulated products in volumes ranging from 300 to 3000 kg annually. For a detailed analysis of import, manufacturing and use of this chemical refer to the NICNAS assessment report for HFE-7100 (NICNAS, 2006).

No specific Australian use, import, or manufacturing information was identified for the remaining chemicals in this group. Information collected by NICNAS in 2006 indicated PFHxA, PFPeA and their derivatives are not currently imported or manufactured in Australia. However, this information could be incomplete because the call for information did not specifically include the PFCAs group (NICNAS, 2013).

It is noted that some of 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. However, release from these uses is beyond the scope of this assessment.

International

The fluorotelomer alcohol and simple methacrylate monomers in this group are used as intermediates in the manufacture of polymers with fluorinated side-chains. In particular, the 6:2 fluorotelomer derivatives have been selected to replace 8:2 fluorotelomer chemistry (Buck, et al., 2011; Zhao, et al., 2013), and therefore are expected to have significant use. Both 6:2 FTOH and 6:2 FTMAC are currently registered for use in Europe, with 6:2 FTMAC reported to be used at 100 to 1000 tonnes per annum (ECHA, 2015). It is noted that these chemicals have also been detected in the final polymer products as residual unreacted starting material (Norden, 2013).

The perfluorotrialkylamines are marketed as speciality chemicals for use in the industrial electronics sector, with principal applications including use as heat transfer agents in semiconductor processing and electronics testing, and as solvents for computer disc drive lubrication (US EPA, 2007). Perfluorotributylamine has also been used as a synthetic oxygen carrier (Kimelman-Bleich, et al., 2009).

The polyfluoroalkyl silane, 1*H*,1*H*,2*H*,2*H*-perfluorohexylmethyldichlorosilane (CAS RN 38436-16-7), may be used as a monomer in polymer production (REACH, 2019). Homologous polyfluoroalkyl silanes are used in cosmetics, spray-on nanofilm surface coatings, and paint lacquers, and they are also used as adhesion promoters between inorganic and fluoropolymer materials (NICNAS, 2018b).

Data available for methoxyperfluorobutane indicate that this chemical is used as a solvent and viscosity control agent in cosmetic products (European Commission, 2013; Norden, 2013).

Limited current data were identified for the remaining chemicals in this group. Available information indicates that the polyfluorinated succinate salt (CAS RN 54950-05-9) may have use as a wetting and levelling agent in emulsions and cleaning products (Ash and Ash, 2004). The polyfluoroalcohol, 1*H*,1*H*,5*H*-octafluoro-1-pentanol (CAS RN 355-80-6), is registered for use as an intermediate in Europe (ECHA, 2015).

Environmental Regulatory Status

Australia

Under Section 65 of the Act, the secondary notification of HFE-7100 (which contains methoxyperfluorobutane (CAS RN 163702-07-6)) may be required where an applicant, or other importer or manufacturer of HFE-7100, becomes aware of any circumstances that may warrant a reassessment of its hazards and risks. Specific circumstances include:

- Manufacture of HFE-7100 has begun, or is likely to begin in Australia.

- Additional information has become available on the adverse health and/or environmental effects of HFE-7100.
- The use of HFE-7100 has changed, or is likely to change significantly.
- The amount of HFE-7100 introduced into Australia has increased, or is likely to increase significantly.

The Director must be notified within 28 days of the introducer becoming aware of any of the above circumstances.

United Nations

The chemicals in this group are not currently identified as Persistent Organic Pollutants (UNEP, 2001), 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, 2013a).

In 2007, methoxyperfluorobutane was identified as a High Production Volume (HPV) chemical by the OECD, indicating that more than 1000 tonnes of the chemical are produced per year in at least one member country (OECD, 2013b). Perfluorotributylamine was also identified as a HPV chemical by the OECD in 2004.

The OECD has been leading an international collaboration on the scientific assessment of, and surveys of, perfluorinated chemicals (OECD, 2018). Since July 2000, Australia has been actively involved in this work through NICNAS.

Canada

Four chemicals in this group, including 6:2 FTOH, the two fluorotelomer methacrylates and methoxyperfluorobutane are listed on the Canadian Domestic Substances List (DSL) (Environment and Climate Change Canada, 2019a). All except methoxyperfluorobutane were categorised during the Categorization of the DSL (Environment and Climate Change Canada, 2019b). One chemical, 6:2 FTOH, was found to be Persistent (P), Bioaccumulative (B), and Inherently Toxic to the Environment (iTE). The two methacrylates were also found to be B and iT_E, but were not found to be P (Environment and Climate Change Canada, 2019b). No subsequent screening assessments have been conducted.

The remaining chemicals in this group are not listed on the DSL (Environment and Climate Change Canada, 2019a). Hexanamide, 2-[2,4-bis(1,1-dimethylpropyl)phenoxy]-*N*-[3-hydroxy-4-[(2,2,3,3,4,4,5,5-octafluoro-1-oxopentyl)amino]phenyl]- (CAS RN 72494-14-5) and hexanamide, 2-[2,4-bis(1,1-dimethylpropyl)phenoxy]-*N*-[4-[(2,2,3,3,4,4,4-heptafluoro-1-oxobutyl)amino]-3-hydroxyphenyl]- (CAS RN 2923-93-5) are listed on the Non-Domestic Substances List (NDSL) and notification under the New Substances Notification Regulations (Chemicals and Polymers) is required before they can be manufactured or imported into Canada above threshold quantities (Environment and Climate Change Canada, 2019a).

European Union

Four chemicals (6:2 FTOH, 6:2 FTMAC, 1*H*,1*H*,2*H*,2*H*-perfluorohexylmethyldichlorosilane and 1*H*,1*H*,5*H*-octafluoro-1-pentanol) in this group are registered for use in the European Union under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation (ECHA, 2015). The monomer, 6:2 FTMAC, is listed on the Community Rolling Action Plan (CoRAP) for evaluation based on a range of concerns which include suspected PBT/vPvB properties, endocrine disruptor potential, and wide-dispersive use (ECHA, 2017a).

Some chemicals in the group (CAS RNs 163702-07-6, 54950-05-9, 311-89-7, 338-84-1, 2923-93-5, and 1799-84-4) were pre-registered for use in the European Union under the REACH legislation (ECHA, 2017b).

United States of America

Perfluorotripentylamine and perfluorotributylamine were identified as HPV chemicals by the United States Environmental Protection Agency (US EPA) in 2010, indicating that they were produced or imported at more than one million pounds (approximately 450 tonnes) per annum (US EPA, 2013).

Environmental Exposure

Some chemicals in this group may be released to the environment as a result of industrial use in Australia. Disposal of cleaning and cosmetic products containing methoxyperfluorobutane to sewer is expected to result in emissions of the chemical to air, surface water and/or landfill. Nevertheless, most other chemicals in this group are not expected to have significant commercial use, as the primary industrial applications identified internationally are not common in Australia.

The environmental degradants of primary concern in this group are the short chain PFCAs (PFHxA, PFPeA and PFBA, and their polyfluorinated analogues). These perfluorinated chemicals are highly resistant to degradation in the environment (NICNAS, 2015c). In the absence of information to the contrary, it is assumed that the polyfluorinated acids are similarly persistent.

Multiple studies have demonstrated the potential for fluorotelomer alcohols to degrade to perfluorocarboxylic acids. Data for 8:2 FTOH demonstrate that homologous fluorotelomer alcohols (FTOHs) will predominantly degrade to perfluorocarboxylic acids by a mechanism which involves the defluorination of one perfluorinated carbon atom (Butt, et al., 2014; De Voogt, 2010; Dinglasan, et al., 2004). Studies of the microbial biodegradation pathway of 6:2 FTOH show that the products of the degradation process include short-chain PFCAs, mainly PFPeA and some PFHxA and PFBA. It is unclear if some of the chemicals detected in these degradation studies, such as 5:3 and 4:3 acids, are final degradation products or intermediates (Kim, et al., 2014; Zhao, et al., 2013). If released to the atmosphere, degradation of FTOHs is expected to occur by a similar mechanism to that proposed for 8:2 FTOH whereby oxidation by chlorine or hydroxyl radicals results in a so-called ‘unzipping’ cycle that forms perfluorinated acids of various lengths (Ellis, et al., 2004).

Data for indirect precursors to other PFCAs, including studies considering substances containing the 8:2 fluorotelomer moiety, indicate that primary degradation of some other chemicals in this group will also release FTOHs into the environment (NICNAS, 2015b). These intermediate products will then undergo subsequent degradation to perfluorocarboxylic acids. Fewer data are available for the more chemically complex PFASs in this group. However, potential degradation of these chemicals to short-chain PFCAs has been assumed (OECD, 2007, 2018).

The environmental fate and behaviour of the polyfluoroalcohol, 1*H*,1*H*,5*H*-octafluoro-1-pentanol (CAS RN 355-80-6), and the three closely related octafluoropentylamide derivatives (CAS RNs 72494-14-5, 83003-52-5, and 97331-50-5) is unknown. However, hydrolysis of each of the three amides would be expected to release the same polyfluorocarboxylic acid: 2,2,3,3,4,4,5,5-octafluoropentanoic acid; CAS RN 376-72-7. The same acid could also be formed by oxidation of the terminal alcohol in 1*H*,1*H*,5*H*-octafluoro-1-pentanol. This acid is a close structural analogue of perfluoropentanoic acid (PFPeA; CAS RN 2706-90-3) and the properties of this short-chain PFCA are taken to be representative of the environmental fate and effects of 2,2,3,3,4,4,5,5-octafluoropentanoic acid for the purposes of this assessment.

Monitoring data have identified 6:2 FTOH and PFHxA in the environment. A study conducted in Canada showed that the volatile 6:2 FTOH is found in outdoor air, in concentrations ranging from 29 picograms per cubic metre (pg/m^3) in a rural environment to 87 pg/m^3 in a highly urbanised location (Martin, et al., 2002). Another study conducted in Germany reported environmental concentrations of 6:2 FTOH in the air ranging from 17 to 149 pg/m^3 (Jahnke, et al., 2007). PFHxA has been detected in Australia in the waters of Sydney Harbour at a concentration of 2.9 nanograms per litre (ng/L) (Thompson, et al., 2011). However, it is noted that there are multiple potential sources for 6:2 FTOH and PFHxA 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.

Environmental Effects

The currently available data for the short-chain PFCAs are summarised in the IMAP Environment Tier II assessment for Short-Chain Perfluorocarboxylic acids and their Direct Precursors (NICNAS, 2015c). Based on data for PFHxA and PFBA, all short-

chain perfluorocarboxylic acids, including PFPeA, were categorised as not Toxic (Not T) according to domestic environmental hazard criteria.

The chemicals in this group contain a range of functional groups and moieties which are correlated with toxic effects in aquatic organisms. In addition, some studies suggest that 6:2 FTOH has (o)estrogenic activity in fish (Ishibashi, et al., 2008; Liu, et al., 2009). Other chemicals in this group have the potential to be long-lived gases in the atmosphere with moderate to high global warming potentials (Hong, et al., 2013; NICNAS, 2006; US EPA, 2007). However, these possible effects have not been considered in this assessment, as the primary risk posed to the environment by the PFASs in this group is assumed to result from the cumulative release of short-chain PFCAs in the environment. The total concentration of PFCAs is expected to be much greater than that of any of the shorter lived precursors.

Categorisation of Environmental Hazard

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

However, the potential degradants PFHxA, PFPeA and PFBA and their direct precursors have been categorised as Persistent, not Bioaccumulative and not Toxic (P, Not B, Not T) (NICNAS, 2015c).

Risk Characterisation

Industrial use of the chemicals in this group is expected to result in environmental emissions. These chemicals may degrade to substances which are extremely persistent and mobile in the environment.

Methoxyperfluorobutane has reported use in cosmetics and a full human health and environmental risk assessment of this chemical is available in the NICNAS assessment report for HFE-7100 (NICNAS, 2006). It was concluded that when this chemical is used in cosmetic products, it is not expected to pose a risk to the aquatic or soil environmental compartments, but will effectively contribute to a very small extent to Australia’s greenhouse gas emissions and probably contribute a similar amount to the global pool of short-chain PFCAs.

It is noted that the perfluoroalkyl carboxylic acid degradants formed from the PFASs in this group may have multiple sources. Due to their persistence in the environment short-chain PFCA levels may continue to increase over time due to indirect release pathways. The scale and time frame of such an increase, and its relevance to characterising the long term environmental risk profile of these perfluoroalkyl carboxylic acids, currently remain unknown.

Key Findings

Based on available domestic and international data, some chemicals in this group may have current industrial use in household products, such as cleaning products and cosmetics. However, most chemicals in this group are expected to have limited industrial use in Australia.

Available data indicate that the PFASs in this group have the potential to degrade to PFHxA, PFPeA and PFBA. Therefore, the principal risk posed by these chemicals is assumed to result from cumulative releases of short-chain perfluorocarboxylic acid degradation products. These perfluoroalkyl carboxylic acids are extremely persistent and mobile and, as a result, they have the potential to become globally distributed environmental contaminants. Nevertheless, currently available data indicate that short-chain PFCAs are not expected to be highly bioaccumulative or toxic to aquatic organisms.

The fate of substances in the environment which have a highly fluorinated alkyl chain terminated with a difluoromethyl group is currently unknown. This is a gap in the available environmental hazard data for highly fluorinated organic chemicals. In the absence of other information, it is assumed that these chemicals will degrade to recalcitrant polyfluorinated organic acids and that they will have similar mobility and persistence in the environment as PFCAs with the same carbon atom chain length. NICNAS may reconsider these assumptions if relevant and reliable studies of the environmental fate of substances which have a highly fluorinated alkyl chain terminated with difluoromethyl group are made available.

The parent 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 available data

to characterise these potential hazards for each individual chemical.

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

Recommendations

The chemicals in this group are not prioritised for further assessment under the IMAP Framework.

However, further assessment may be necessary if information becomes available indicating the use pattern and/or introduction volume of the chemicals in this group are significantly different to that considered in this report, or if information becomes available indicating adverse effects on the environment from either the parent chemicals or their principal degradation products.

It is noted that the IMAP Environment Tier II Assessment for Short-Chain Perfluorocarboxylic Acids and their Direct Precursors found that sufficient information was available to demonstrate that short-chain perfluorocarboxylic acids have a lower toxicity profile compared to PFOA, and it was recommended that the assessment be included in the NICNAS action plan (NICNAS, 2018a). This should be considered during the application of the action plan to any chemicals which may degrade to short-chain perfluorocarboxylic acids.

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 the PFHxA degradant that can be formed from some of the chemicals in this group has been classified as Acute Aquatic Category 3 (H402: Harmful to aquatic life) under the GHS (NICNAS, 2015c).

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