# Indirect precursors to perfluoroalkyl sulfonates: Environment tier II assessment

**03 July 2015**

## CAS Registry Number: 68555-74-8, 68555-72-6, 68298-06-6, 68555-75-9, 34455-03-3, 1893-52-3, 68555-76-0, 68555-73-7, 59071-10-2, 68957-60-8, 68957-55-1, 68957-57-3, 68957-61-9, 52166-82-2, 68957-58-4, 73772-32-4, 81190-38-7, 38850-58-7, 67940-02-7, 68555-81-7, 67584-58-1, 67584-52-5, 67584-53-6, 67584-62-7, 67939-90-6, 67969-65-7, 67923-61-9, 67939-98-4, 67939-97-3, 67939-94-0, 68298-80-6, 68310-17-8, 56372-23-7, 68259-38-1, 68298-81-7, 68958-60-1, 68259-39-2, 68541-02-6, 68891-99-6, 68815-72-5, 68891-98-5, 68541-01-5, 68891-97-4




## 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 the new 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 a group of 43 chemicals. The chemicals in this group are structurally related compounds in that they all contain a chain of either five, six or seven perfluorinated carbons linked to a terminal sulfonamide or sulfonic ester group.

NICNAS has developed an action plan to assess and manage chemicals which may degrade to perfluorinated carboxylic acids, perfluoroalkyl sulfonates and similar chemicals, which can be found in Appendix G of the Handbook for Notifiers on the NICNAS website (NICNAS, 2015d). The primary assumption outlined in this action plan is that chemicals with a perfluorinated chain terminated by a sulfonyl group will degrade to the perfluoroalkyl sulfonate (of the same chain length). On this basis the chemicals in this group are expected to degrade to form the $C_5$ perfluoropentanesulfonate anion (PFPeS), the $C_6$ perfluorohexanesulfonate anion (PFHxS), or the $C_7$ perfluoroheptanesulfonate anion (PFHpS) in the aquatic environment.

The perfluorinated anions that can be released by the chemicals in this group have chain lengths which are intermediate to the homologous $C_4$ perfluorobutanesulfonate anion (PFBS) and the $C_8$ perfluorooctanesulfonate anion (PFOS). Data currently available for simple salts of PFBS indicate that although this short-chain anion is exceptionally persistent in the environment, it is not bioaccumulative or toxic (NICNAS, 2015e). However, the long-chain PFOS anion is persistent, bioaccumulative, and toxic,

and substances which release this anion are considered to pose a significant hazard both to human health and the environment (NICNAS, 2015a).

Degradation of the $C_5$ to $C_7$ perfluoroalkyl sulfonate anions is very slow compared with their rate of formation from the degradation of their precursors. Therefore, the concentration of $C_5$ to $C_7$ perfluoroalkyl sulfonate anions in the environment is expected to be higher than that of any of their respective precursors. It will therefore be assumed for the purposes of this assessment that the primary risk posed by the chemicals in this group results from the release of the $C_5$ to $C_7$ perfluoroalkyl sulfonate anions to the environment. The IMAP Environment Tier II assessment for Direct Precursors to Perfluoroheptanesulfonate (PFHpS), Perfluorohexanesulfonate (PFHxS) and Perfluoropentanesulfonate (PFPeS) has been used as a reference assessment (NICNAS, 2015b).

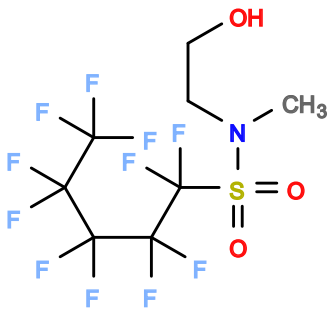
## Chemical Identity

In this assessment, “PFHpS” is used to denote the conjugate base anion of perfluoroheptanesulfonic acid (i.e. the perfluoroheptanesulfonate anion), “PFHxS” is used to denote the conjugate base anion of perfluorohexanesulfonic acid (i.e. the perfluorohexanesulfonate anion), and “PFPeS” is used to denote the conjugate base anion of perfluoropentanesulfonic acid (i.e. the perfluoropentanesulfonate anion) (Buck, et al., 2011).

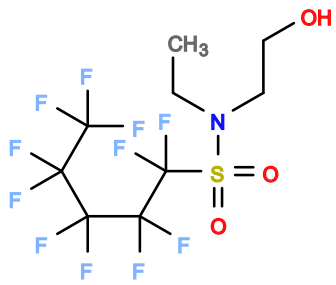
Acronyms for certain chemicals in this group have been taken from a list of recommended acronyms and other terminology recently compiled to facilitate clear and unambiguous communication regarding the major classes of industrially important perfluoroalkyl and polyfluoroalkyl substances (Buck, et al.,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

This assessment includes a range of neutral and ionic organic chemicals. For purposes of presentation the chemicals in this assessment have been sub-grouped below based on similar structural properties and their perfluorinated chain length.

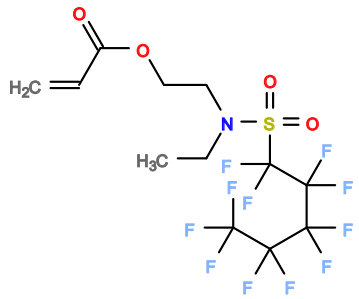
## Neutral Organic Derivatives of Perfluoropentanesulfonamides

| | |
|---|---|
| CAS RN | 68555-74-8 |
| Chemical Name | 1-Pentanesulfonamide, 1,1,2,2,3,3,4,4,5,5,5-undecafluoro-*N*-(2-hydroxyethyl)-*N*-methyl- |
| Synonyms | MeFPeSE<br>*N*-methylperfluoropentanesulfonamidoethanol |
| Structural Formula |  |

| | |
|---|---|
| Molecular Formula | $C_8H_8F_{11}NO_3S$ |
| Molecular Weight (g/mol) | 407.20 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(C)CCO |

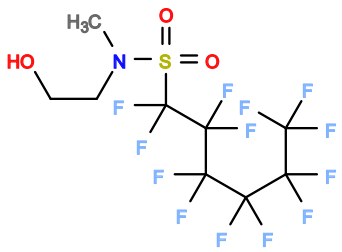
| | |
|---|---|
| CAS RN | 68555-72-6 |
| Chemical Name | 1-Pentanesulfonamide, *N*-ethyl-1,1,2,2,3,3,4,4,5,5,5-undecafluoro-*N*-(2-hydroxyethyl)- |
| Synonyms | EtFPeSE<br>*N*-ethylperfluoropentanesulfonamidoethanol |
| Structural Formula |  |
| Molecular Formula | $C_9H_{10}F_{11}NO_3S$ |
| Molecular Weight (g/mol) | 421.23 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCO)CC |

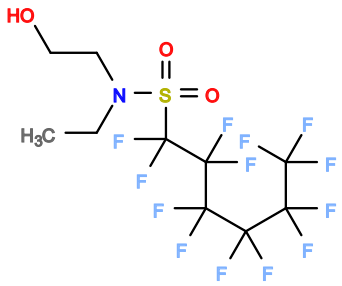
| | |
|---|---|
| CAS RN | 68298-06-6 |

| | |
|---|---|
| Chemical Name | 2-Propenoic acid, 2-[ethyl[(1,1,2,2,3,3,4,4,5,5,5-undecafluoropentyl)sulfonyl]amino]ethyl ester |
| Synonyms | EtFPeSAC<br>*N*-ethylperfluoropentanesulfonamindoethyl acrylate |
| Structural Formula |  |
| Molecular Formula | $C_{12}H_{12}F_{11}NO_4S$ |
| Molecular Weight (g/mol) | 475.28 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOC(=O)C=C)CC |

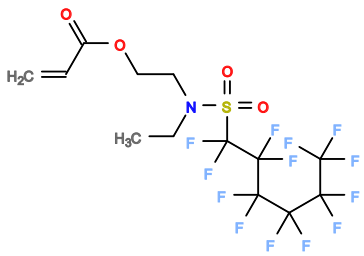
## Neutral Organic Derivatives of Perfluorohexanesulfonamides

| | |
|---|---|
| CAS RN | 68555-75-9 |
| Chemical Name | 1-Hexanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-*N*-(2-hydroxyethyl)-*N*-methyl- |
| Synonyms | MeFHxSE<br>*N*-methylperfluorohexanesulfonamidoethanol |
| Structural Formula | |

| | |
|---|---|
| |  |
| Molecular Formula | $C_9H_8F_{13}NO_3S$ |
| Molecular Weight (g/mol) | 457.21 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(C)CCO |

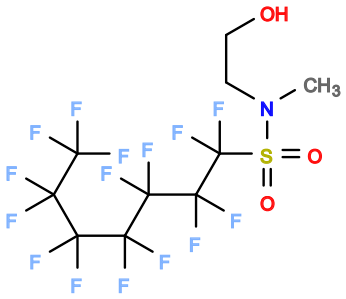
| | |
|---|---|
| CAS RN | 34455-03-3 |
| Chemical Name | 1-Hexanesulfonamide, *N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-*N*-(2-hydroxyethyl)- |
| Synonyms | EtFHxSE<br>*N*-ethylperfluorohexanesulfonamidoethanol |
| Structural Formula |  |
| Molecular Formula | $C_{10}H_{10}F_{13}NO_3S$ |
| Molecular Weight (g/mol) | 471.24 |

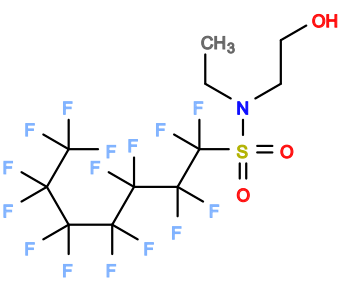
| | |
|---|---|
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCO)CC |

| | |
|---|---|
| CAS RN | 1893-52-3 |
| Chemical Name | 2-Propenoic acid, 2-[ethyl[(tridecafluorohexyl)sulfonyl]amino]ethyl ester |
| Synonyms | EtFHxSAC<br>*N*-ethylperfluorohexanesulfonamindoethyl acrylate |
| Structural Formula |  |
| Molecular Formula | $C_{13}H_{12}F_{13}NO_4S$ |
| Molecular Weight (g/mol) | 525.28 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOC(=O)C=C)CC |

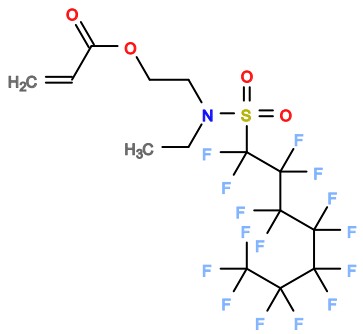
## Neutral Organic Derivatives of Perfluoroheptanesulfonamides

| | |
|---|---|
| CAS RN | 68555-76-0 |
| Chemical Name | 1-Heptanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-*N*-(2-hydroxyethyl)-*N*-methyl- |

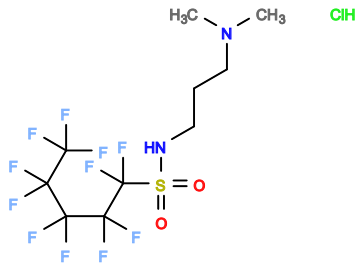
| | |
|---|---|
| Synonyms | MeFHpSE<br><br>*N*-methylperfluoroheptanesulfonamidoethanol |
| Structural Formula |  |
| Molecular Formula | $C_{10}H_8F_{15}NO_3S$ |
| Molecular Weight (g/mol) | 507.22 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(C)CCO |

| | |
|---|---|
| CAS RN | 68555-73-7 |
| Chemical Name | 1-Heptanesulfonamide, *N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-*N*-(2-hydroxyethyl)- |
| Synonyms | EtFHpSE<br><br>*N*-ethylperfluoroheptanesulfonamidoethanol |
| Structural Formula |  |

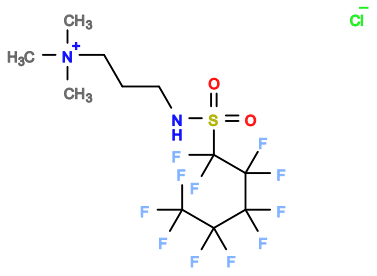
| | |
|---|---|
| Molecular Formula | $C_{11}H_{10}F_{15}NO_3S$ |
| Molecular Weight (g/mol) | 521.24 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCO)CC |

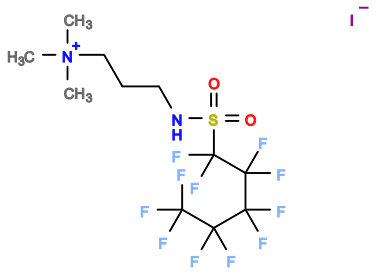
| | |
|---|---|
| CAS RN | 59071-10-2 |
| Chemical Name | 2-Propenoic acid, 2-[ethyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl ester |
| Synonyms | EtFHpSAC<br>*N*-ethylperfluoroheptanesulfonamindoethyl acrylate |
| Structural Formula |  |
| Molecular Formula | $C_{14}H_{12}F_{15}NO_4S$ |
| Molecular Weight (g/mol) | 575.29 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOC(=O)C=C)CC |

# Alkyl Ammonium and Amine Derivatives of Perfluoropentanesulfonamides

| | |
|---|---|
| CAS RN | 68957-60-8 |
| Chemical Name | 1-Pentanesulfonamide, *N*-[3-(dimethylamino)propyl]-1,1,2,2,3,3,4,4,5,5,5-undecafluoro-, monohydrochloride |
| Synonyms | *N*-(3-(dimethylaminopropyl)perfluoropentanesulfonamide monohydrochloride |
| Structural Formula |  |
| Molecular Formula | $C_{10}H_{14}ClF_{11}N_2O_2S$ |
| Molecular Weight (g/mol) | 470.73 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)NCCCN(C)C.Cl |

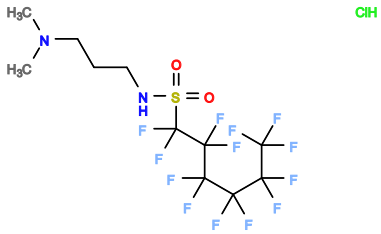
| | |
|---|---|
| CAS RN | 68957-55-1 |
| Chemical Name | 1-Propanaminium, *N*,*N*,*N*-trimethyl-3-[[(undecafluoropentyl)sulfonyl]amino]-, chloride |
| Synonyms | *N*-(3-(trimethyl)aminopropyl)perfluoropentanesulfonamide chloride |
| Structural Formula | |

| | |
|---|---|
| |  |
| Molecular Formula | $C_{11}H_{16}ClF_{11}N_2O_2S$ |
| Molecular Weight (g/mol) | 484.76 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)NCCC[N+](C)(C)C.[Cl-] |

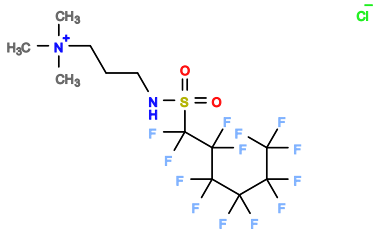
| | |
|---|---|
| CAS RN | 68957-57-3 |
| Chemical Name | 1-Propanaminium, *N*,*N*,*N*-trimethyl-3-[[(undecafluoropentyl)sulfonyl]amino]-, iodide |
| Synonyms | *N*-(3-(trimethyl)aminopropyl)perfluoropentanesulfonamide iodide |
| Structural Formula |  |
| Molecular Formula | $C_{11}H_{16}F_{11}IN_2O_2S$ |
| Molecular Weight (g/mol) | 576.21 |
| | |

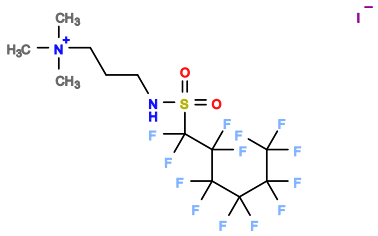
| | |
|---|---|
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)NCCC[N+](C)(C)C.[I-] |

## Alkyl Ammonium and Amine Derivatives of Perfluorohexanesulfonamides

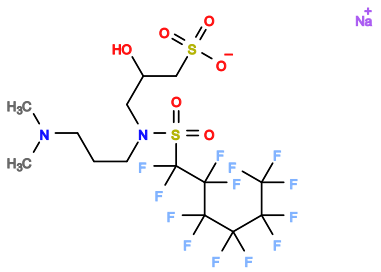
| | |
|---|---|
| CAS RN | 68957-61-9 |
| Chemical Name | 1-Hexanesulfonamide, *N*-[3-(dimethylamino)propyl]-1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-, monohydrochloride |
| Synonyms | *N*-(3-(dimethylaminopropyl)perfluorohexanesulfonamide monohydrochloride |
| Structural Formula |  |
| Molecular Formula | $C_{11}H_{14}ClF_{13}N_2O_2S$ |
| Molecular Weight (g/mol) | 520.74 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)NCCCN(C)C.Cl |

| | |
|---|---|
| CAS RN | 52166-82-2 |
| Chemical Name | 1-Propanaminium, *N*,*N*,*N*-trimethyl-3-[[(tridecafluorohexyl)sulfonyl]amino]-, chloride |
| Synonyms | *N*-(3-(trimethyl)aminopropyl)perfluorohexanesulfonamide chloride |

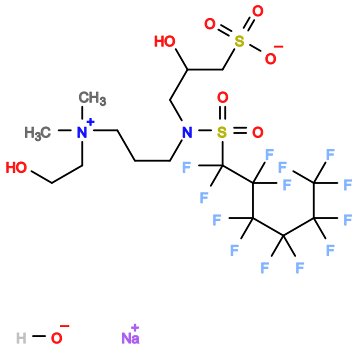
| | |
|---|---|
| Structural Formula |  |
| Molecular Formula | $C_{12}H_{16}ClF_{13}N_2O_2S$ |
| Molecular Weight (g/mol) | 534.76 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)NCCC[N+](C)(C)C.[Cl-] |

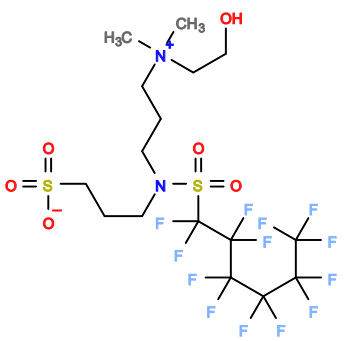
| | |
|---|---|
| CAS RN | 68957-58-4 |
| Chemical Name | 1-Propanaminium, *N*,*N*,*N*-trimethyl-3-[[(tridecafluorohexyl)sulfonyl]amino]-, iodide |
| Synonyms | *N*-(3-(trimethyl)aminopropyl)perfluorohexanesulfonamide iodide |
| Structural Formula |  |
| Molecular Formula | $C_{12}H_{16}F_{13}IN_2O_2S$ |
| Molecular Weight (g/mol) | 626.22 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)NCCC[N+](C) |

| | |
|---|---|
| | (C)C.[I-] |

| | |
|---|---|
| CAS RN | 73772-32-4 |
| Chemical Name | 1-Propanesulfonic acid, 3-[[3-(dimethylamino)propyl] [(tridecafluorohexyl)sulfonyl]amino]-2-hydroxy-, monosodium salt |
| Synonyms | sodium *N*-(3-(dimethyl)aminoproply)perfluorohexanesulfonamide 2-hydroxypropyl sulfonate |
| Structural Formula |  |
| Molecular Formula | $C_{14}H_{18}F_{13}N_2NaO_6S_2$ |
| Molecular Weight (g/mol) | 644.40 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CC(O)CS(=O)(=O)[O-])CCCN(C)C.[Na+] |

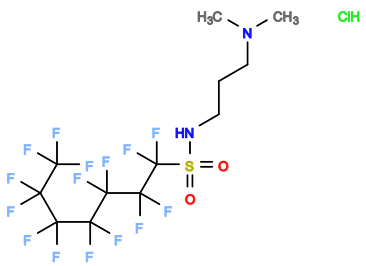
| | |
|---|---|
| CAS RN | 81190-38-7 |
| Chemical Name | 1-Propanaminium, *N*-(2-hydroxyethyl)-3-[(2-hydroxy-3-sulfopropyl) [(tridecafluorohexyl)sulfonyl]amino]-*N*,*N*-dimethyl-, hydroxide, monosodium salt |
| Synonyms | sodium *N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-3-[(2-hydroxy-3-sulfopropyl)perfluorohexane sulfonamino]propylammonium hydroxide |

| | |
|---|---|
| Structural Formula |  |
| Molecular Formula | $C_{16}H_{24}F_{13}N_2NaO_8S_2$ |
| Molecular Weight (g/mol) | 706.47 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CC(O)CS(=O)(=O)[O-])CCC[N+](C)(C)CCO.[Na+].[OH-] |

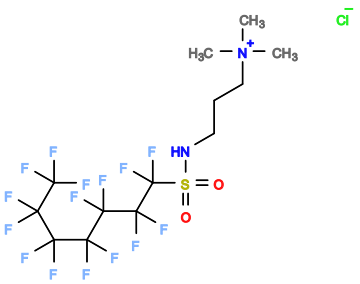
| | |
|---|---|
| CAS RN | 38850-58-7 |
| Chemical Name | 1-Propanaminium, *N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-3-[(3-sulfopropyl)[(tridecafluorohexyl)sulfonyl]amino]-, hydroxide, inner salt |
| Synonyms | *N*-(3-(dimethyl)(hydroxyethyl)aminopropyl)perfluorohexanesulfonamide propylsulfate, inner salt |
| Structural Formula |  |
| Molecular Formula | $C_{16}H_{23}F_{13}N_2O_6S_2$ |

| | |
|---|---|
| Molecular Weight (g/mol) | 650.47 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCC[N+](C)(C)CCO)CCCS(=O)(=O)[O-] |

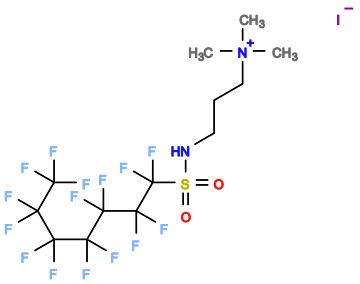
## Alkyl Ammonium and Amine Derivatives of Perfluoroheptanesulfonamides

| | |
|---|---|
| CAS RN | 67940-02-7 |
| Chemical Name | 1-Heptanesulfonamide, *N*-[3-(dimethylamino)propyl]-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-, monohydrochloride |
| Synonyms | *N*-(3-(dimethylaminopropyl)perfluoroheptanesulfonamide monohydrochloride |
| Structural Formula |  |
| Molecular Formula | $C_{12}H_{14}ClF_{15}N_2O_2S$ |
| Molecular Weight (g/mol) | 570.75 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)NCCCN(C)C.Cl |

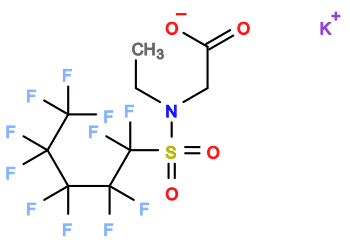
| | |
|---|---|
| CAS RN | 68555-81-7 |

| | |
|---|---|
| Chemical Name | 1-Propanaminium, *N*,*N*,*N*-trimethyl-3-[[(pentadecafluoroheptyl)sulfonyl]amino]-, chloride |
| Synonyms | *N*-(3-(trimethyl)aminopropyl)perfluoroheptanesulfonamide chloride |
| Structural Formula |  |
| Molecular Formula | $C_{13}H_{16}ClF_{15}N_2O_2S$ |
| Molecular Weight (g/mol) | 584.77 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)NCCC[N+](C)(C)C.[Cl-] |

| | |
|---|---|
| CAS RN | 67584-58-1 |
| Chemical Name | 1-Propanaminium, *N*,*N*,*N*-trimethyl-3-[[(pentadecafluoroheptyl)sulfonyl]amino]-, iodide |
| Synonyms | *N*-(3-(trimethyl)aminopropyl)perfluoroheptanesulfonamide iodide |
| Structural Formula | |

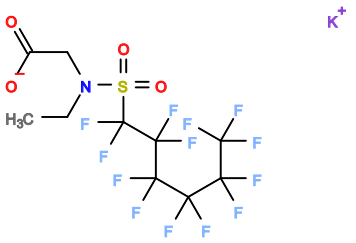
| | |
|---|---|
| |  |
| Molecular Formula | $C_{13}H_{16}F_{15}IN_2O_2S$ |
| Molecular Weight (g/mol) | 676.22 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)NCCC[N+](C)(C)C.[I-] |

## Carboxylic acid Derivatives of Perfluoropentanesulfonamides

| | |
|---|---|
| CAS RN | 67584-52-5 |
| Chemical Name | Glycine, *N*-ethyl-*N*-[(undecafluoropentyl) sulfonyl]-, potassium salt |
| Synonyms | potassium *N*-ethylperfluoropentanesulfonamido acetate |
| Structural Formula |  |
| Molecular Formula | $C_9H_7F_{11}KNO_4S$ |
| Molecular Weight (g/mol) | 473.30 |

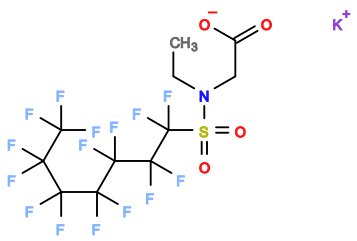
| | |
|---|---|
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CC(=O)[O-])CC.[K+] |

## Carboxylic acid Derivatives of Perfluorohexanesulfonamides

| | |
|---|---|
| CAS RN | 67584-53-6 |
| Chemical Name | Glycine, *N*-ethyl-*N*-[(tridecafluorohexyl)sulfonyl]-, potassium salt |
| Synonyms | potassium EtFHxSAA<br>potassium *N*-ethylperfluorohexanesulfonamido acetate |
| Structural Formula |  |
| Molecular Formula | $C_{10}H_7F_{13}KNO_4S$ |
| Molecular Weight (g/mol) | 523.31 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CC(=O)[O-])CC.[K+] |

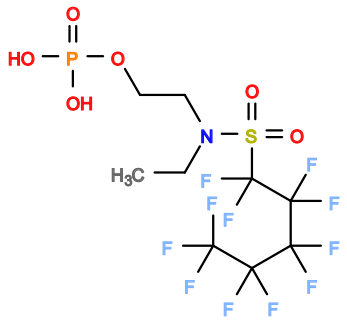
## Carboxylic acid Derivatives of Perfluoroheptanesulfonamides

| | |
|---|---|
| CAS RN | 67584-62-7 |
| | |

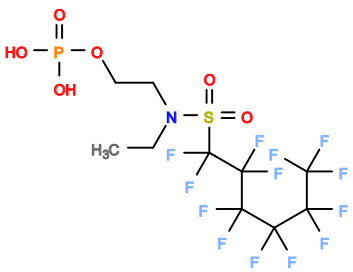
| | |
|---|---|
| Chemical Name | Glycine, *N*-ethyl-*N*-[(pentadecafluoroheptyl)sulfonyl]-, potassium salt |
| Synonyms | potassium EtFHpSAA<br>potassium *N*-ethylperfluoroheptanesulfonamido acetate |
| Structural Formula |  |
| Molecular Formula | $C_{11}H_7F_{15}KNO_4S$ |
| Molecular Weight (g/mol) | 573.32 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CC(=O)[O-])CC.[K+] |

## Phosphate Esters of Perfluoropentanesulfonamides

| | |
|---|---|
| CAS RN | 67939-90-6 |
| Chemical Name | 1-Pentanesulfonamide, *N*-ethyl-1,1,2,2,3,3,4,4,5,5,5-undecafluoro-*N*-[2-(phosphonooxy)ethyl]- |
| Synonyms | *N*-ethylperfluoropentanesulfonamidoethyl dihydrogen phosphate |
| Structural Formula | |

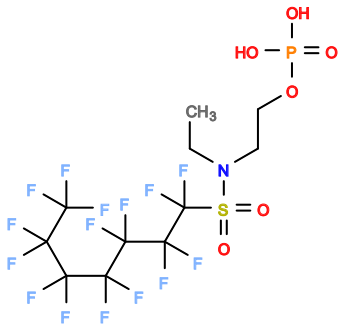
| | |
|---|---|
| |  |
| Molecular Formula | $C_9H_{11}F_{11}NO_6PS$ |
| Molecular Weight (g/mol) | 501.21 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOP(=O)(O)O)CC |

## Phosphate Esters of Perfluorohexanesulfonamides

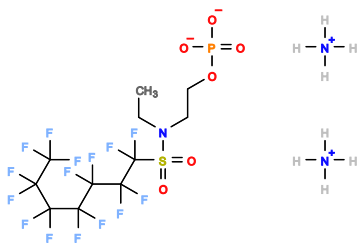
| | |
|---|---|
| CAS RN | 67969-65-7 |
| Chemical Name | 1-Hexanesulfonamide, *N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-*N*-[2-(phosphonooxy)ethyl]- |
| Synonyms | *N*-ethylperfluorohexanesulfonamidoethyl dihydrogen phosphate |
| Structural Formula |  |
| Molecular Formula | $C_{10}H_{11}F_{13}NO_6PS$ |

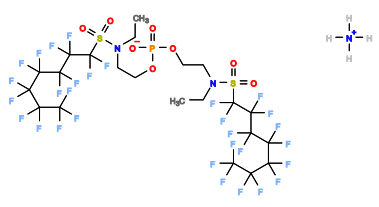
| | |
|---|---|
| Molecular Weight (g/mol) | 551.22 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOP(=O)(O)O)CC |

## Phosphate Esters of Perfluoroheptanesulfonamides

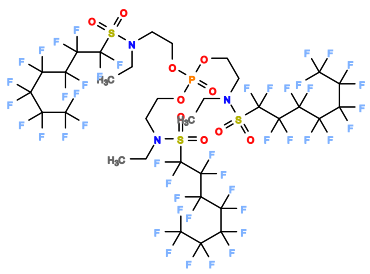
| | |
|---|---|
| CAS RN | 67923-61-9 |
| Chemical Name | 1-Heptanesulfonamide, *N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-*N*-[2-(phosphonooxy)ethyl]- |
| Synonyms | *N*-ethylperfluoroheptanesulfonamidoethyl dihydrogen phosphate |
| Structural Formula |  |
| Molecular Formula | $C_{11}H_{11}F_{15}NO_6PS$ |
| Molecular Weight (g/mol) | 601.22 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOP(=O)(O)O)CC |

| | |
|---|---|
| CAS RN | 67939-98-4 |

| | |
|---|---|
| Chemical Name | 1-Heptanesulfonamide, *N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-*N*-[2-(phosphonooxy)ethyl]-, diammonium salt |
| Synonyms | diammonium *N*-ethylperfluoroheptanesulfonamidoethyl phosphate |
| Structural Formula |  |
| Molecular Formula | $C_{11}H_{17}F_{15}N_3O_6PS$ |
| Molecular Weight (g/mol) | 635.28 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOP(=O)([O-])[O-])CC.[NH4+].[NH4+] |

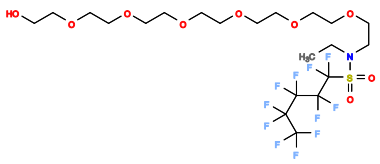
| | |
|---|---|
| CAS RN | 67939-97-3 |
| Chemical Name | 1-Heptanesulfonamide, *N*,*N*'-[phosphinicobis(oxy-2,1-ethanediyl)]bis[*N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-, ammonium salt |
| Synonyms | ammonium bis(*N*-ethylperfluoroheptanesulfonaminoethyl)phosphate |
| Structural Formula |  |
| Molecular Formula | $C_{22}H_{22}F_{30}N_3O_8PS_2$ |

| | |
|---|---|
| Molecular Weight (g/mol) | 1121.48 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOP(=O)([O-])OCCN(CC)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)CC.[NH4+] |

| | |
|---|---|
| CAS RN | 67939-94-0 |
| Chemical Name | 1-Heptanesulfonamide, *N*,*N*',*N*''-[phosphinylidynetris(oxy-2,1-ethanediyl)]tris[*N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro- |
| Synonyms | tris(*N*-ethylperfluoroheptanesulfonaminoethyl)phosphate |
| Structural Formula |  |
| Molecular Formula | $C_{33}H_{27}F_{45}N_3O_{10}PS_3$ |
| Molecular Weight (g/mol) | 1607.68 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOP(=O)(OCCN(CC)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)OCCN(CC)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)CC |

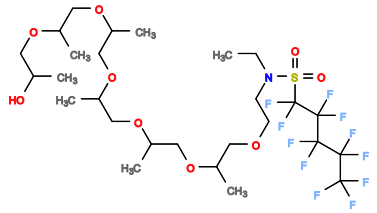
## Polyglycol Derivatives of Perfluoropentanesulfonamides

The substance represented by CAS RN 68298-80-6 is a mixture of discrete chemicals. Representative chemical identity information is provided. However, it should be noted that this substance is expected to include a mixture of chemicals with polyethylene glycol chains of various lengths.

| | |
|---|---|
| CAS RN | 68298-80-6 |
| Chemical Name | Poly(oxy-1,2-ethanediyl), .alpha.-[2-[ethyl[(undecafluoropentyl)sulfonyl]amino]ethyl]-.omega.-hydroxy- |
| Synonyms | *N*-ethylperfluoropentanesulfonamide poly(ethylene glycol) |
| Structural Formula |  |
| Molecular Formula | $C_{21}H_{34}F_{11}NO_9S$ |
| Molecular Weight (g/mol) | 685.55 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOCCOCCOCCOCCOCCOCCO)CC |

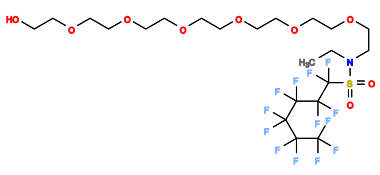
The substance represented by CAS RN 68310-17-8 is a mixture of discrete chemicals. Representative chemical identity information is provided. However, it should be noted that this substance is expected to include a mixture of chemicals with polypropylene glycol chains of various lengths.

| | |
|---|---|
| CAS RN | 68310-17-8 |
| Chemical Name | Poly[oxy(methyl-1,2-ethanediyl)], .alpha.-[2-[ethyl[(undecafluoropentyl)sulfonyl]amino]ethyl]-.omega.-hydroxy- |
| Synonyms | *N*-ethylperfluoropentanesulfonamide poly(propylene glycol) |
| Structural Formula | |

| | |
|---|---|
| |  |
| Molecular Formula | $C_{27}H_{46}F_{11}NO_9S$ |
| Molecular Weight (g/mol) | 769.71 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOCC(C)OCC(C)OCC(C)OCC(C)OCC(C)OCC(C)O)CC |

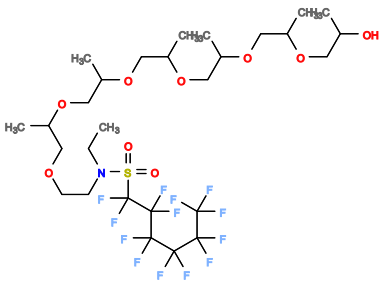
## Polyglycol Derivatives of Perfluorohexanesulfonamides

The substance represented by CAS RN 56372-23-7 is a mixture of discrete chemicals. Representative chemical identity information is provided. However, it should be noted that this substance is expected to include a mixture of chemicals with polyethylene glycol chains of various lengths.

| | |
|---|---|
| CAS RN | 56372-23-7 |
| Chemical Name | Poly(oxy-1,2-ethanediyl), .alpha.-[2-[ethyl[(1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluorohexyl)sulfonyl]amino]ethyl]-.omega.-hydroxy- |
| Synonyms | *N*-ethylperfluorohexanesulfonamide poly(ethylene glycol) |
| Structural Formula |  |
| Molecular Formula | $C_{22}H_{34}F_{13}NO_9S$ |
| Molecular Weight (g/mol) | 735.56 |

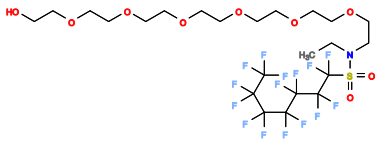
| | |
|---|---|
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOCCOCCOCCOCCOCCOCCO)CC |

The substance represented by CAS RN 68259-38-1 is a mixture of discrete chemicals. Representative chemical identity information is provided. However, it should be noted that this substance is expected to include a mixture of chemicals with polypropylene glycol chains of various lengths.

| | |
|---|---|
| CAS RN | 68259-38-1 |
| Chemical Name | Poly[oxy(methyl-1,2-ethanediyl)], .alpha.-[2-[ethyl[(tridecafluorohexyl)sulfonyl]amino]ethyl]-.omega.-hydroxy- |
| Synonyms | *N*-ethylperfluorohexanesulfonamide poly(propylene glycol) |
| Structural Formula |  |
| Molecular Formula | $C_{28}H_{46}F_{13}NO_9S$ |
| Molecular Weight (g/mol) | 819.72 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOCC(C)OCC(C)OCC(C)OCC(C)OCC(C)OCC(C)O)CC |

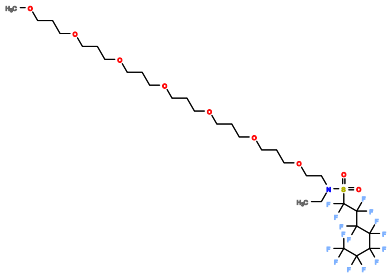
## Polyglycol Derivatives of Perfluoroheptanesulfonamides

The substance represented by CAS RN 68298-81-7 is a mixture of discrete chemicals. Representative chemical identity information is provided. However, it should be noted that this substance is expected to include a mixture of chemicals with polyethylene glycol chains of various lengths.

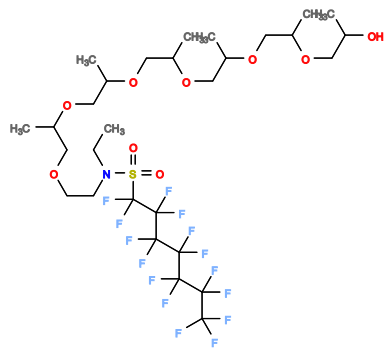
| | |
|---|---|
| CAS RN | 68298-81-7 |
| Chemical Name | Poly(oxy-1,2-ethanediyl), .alpha.-[2-[ethyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl]-.omega.-hydroxy- |
| Synonyms | *N*-ethylperfluoroheptanesulfonamide poly(ethylene glycol) |
| Structural Formula |  |
| Molecular Formula | $C_{23}H_{34}F_{15}NO_9S$ |
| Molecular Weight (g/mol) | 785.56 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOCCOCCOCCOCCOCCOCCO)CC |

The substance represented by CAS RN 68958-60-1 is a mixture of discrete chemicals. Representative chemical identity information is provided. However, it should be noted that this substance is expected to include a mixture of chemicals with polyethylene glycol chains of various lengths.

| | |
|---|---|
| CAS RN | 68958-60-1 |
| Chemical Name | Poly(oxy-1,2-ethanediyl), .alpha.-[2-[ethyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl]-.omega.-methoxy- |
| Synonyms | *N*-ethylperfluoroheptanesulfonamide poly(ethylene glycol) methyl ether |
| Structural Formula | |

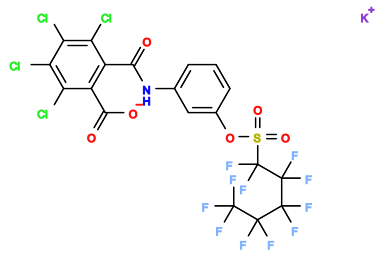
| | |
|---|---|
| |  |
| Molecular Formula | $C_{30}H_{48}F_{15}NO_9S$ |
| Molecular Weight (g/mol) | 883.75 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOCCCOCCCOCCCOCCCOCCCOCCCOC)CC |

The substance represented by CAS RN 68259-39-2 is a mixture of discrete chemicals. Representative chemical identity information is provided. However, it should be noted that this substance is expected to include a mixture of chemicals with polypropylene glycol chains of various lengths.

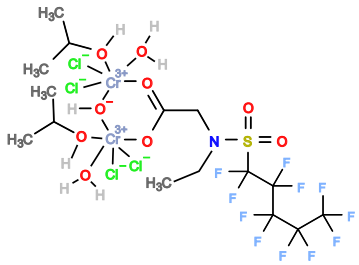
| | |
|---|---|
| CAS RN | 68259-39-2 |
| Chemical Name | Poly[oxy(methyl-1,2-ethanediyl)], .alpha.-[2-[ethyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl]-.omega.-hydroxy- |
| Synonyms | *N*-ethylperfluoroheptanesulfonamide poly(propylene glycol) |
| Structural Formula |  |
| Molecular Formula | $C_{29}H_{46}F_{15}NO_9S$ |

| | |
|---|---|
| Molecular Weight (g/mol) | 869.72 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CCOCC(C)OCC(C)OCC(C)OCC(C)OCC(C)OCC(C)O)CC |

## Miscellaneous Perfluoropentanesulfonyl Derivatives

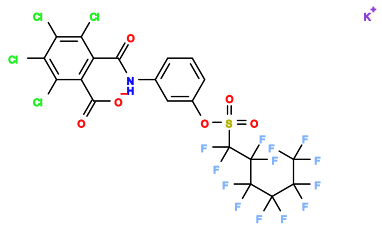
| | |
|---|---|
| CAS RN | 68541-02-6 |
| Chemical Name | Benzoic acid, 2,3,4,5-tetrachloro-6-[[[3-[[(undecafluoropentyl)sulfonyl]oxy]phenyl]amino]carbonyl]-, monopotassium salt |
| Synonyms | potassium 2,3,4,5-tetrachloro-6-[[[3-[[perfluoropentane sulfonyl]oxy]phenyl]amino]carbonyl]benzoate |
| Structural Formula |  |
| Molecular Formula | $C_{19}H_5Cl_4F_{11}KNO_6S$ |
| Molecular Weight (g/mol) | 765.20 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)Oc1cc(NC(=O)c2c(C(=O)[O-])c(Cl)c(Cl)c(Cl)c2Cl)ccc1.[K+] |

The substance represented by CAS RN 68891-99-6 is a dinuclear coordination complex of chromium. The chromium ions in this complex are present in the 3+ oxidation state.

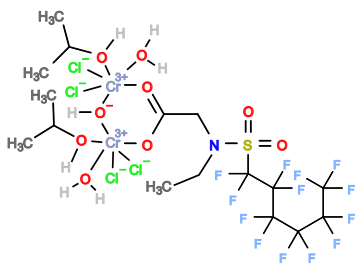
| | |
|---|---|
| CAS RN | 68891-99-6 |
| Chemical Name | Chromium, diaquatetrachloro[.mu.-[*N*-ethyl-*N*-[(undecafluoropentyl)sulfonyl]glycinato-O1:O1']]-.mu.-hydroxybis(2-propanol)di- |
| Synonyms | *N*-ethylperfluoropentanesulfonylamido acetate chromium complex |
| Structural Formula |  |
| Molecular Formula | $C_{15}H_{28}Cl_4Cr_2F_{11}NO_9S$ |
| Molecular Weight (g/mol) | 853.25 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CC1O[Cr+++]([OH]C(C)C)([OH2])([Cl-])([Cl-])[OH-][Cr+++]([OH2])([OH]C(C)C)([Cl-])([Cl-])O=1)CC |

## Miscellaneous Perfluorohexanesulfonyl Derivatives

| | |
|---|---|
| CAS RN | 68815-72-5 |
| Chemical Name | Benzoic acid, 2,3,4,5-tetrachloro-6-[[[3-[[(tridecafluorohexyl)sulfonyl]oxy]phenyl]amino]carbonyl]-, monopotassium salt |
| Synonyms | potassium 2,3,4,5-tetrachloro-6-[[[3-[[perfluorohexane |

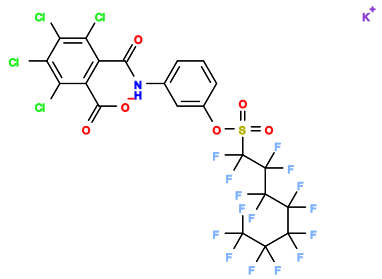
| | |
|---|---|
| | sulfonyl]oxy]phenyl]amino]carbonyl]benzoate |
| Structural Formula |  |
| Molecular Formula | $C_{20}H_5Cl_4F_{13}KNO_6S$ |
| Molecular Weight (g/mol) | 815.21 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)Oc1cc(NC(=O)c2c(C(=O)[O-])c(Cl)c(Cl)c(Cl)c2Cl)ccc1.[K+] |

The substance represented by CAS RN 68891-98-5 is a dinuclear coordination complex of chromium. The chromium ions in this complex are present in the 3+ oxidation state.

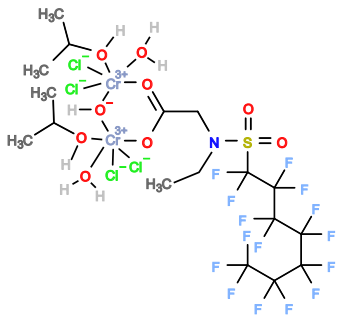
| | |
|---|---|
| CAS RN | 68891-98-5 |
| Chemical Name | Chromium, diaquatetrachloro[.mu.-[*N*-ethyl-*N*-[(tridecafluorohexyl)sulfonyl]glycinato-O1:O1']]-.mu.-hydroxybis[2-propanol]di- |
| Synonyms | *N*-ethylperfluorohexanesulfonamido acetate chromium complex |
| Structural Formula |  |
| Molecular Formula | $C_{16}H_{28}Cl_4Cr_2F_{13}NO_9S$ |

| | |
|---|---|
| Molecular Weight (g/mol) | 903.24 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CC1O[Cr+++]([OH]C(C)C)([OH2])([Cl-])([Cl-])[OH-][Cr+++]([OH2])([OH]C(C)C)([Cl-])([Cl-])O=1)CC |

## Miscellaneous Perfluoroheptanesulfonyl Derivatives

| | |
|---|---|
| CAS RN | 68541-01-5 |
| Chemical Name | Benzoic acid, 2,3,4,5-tetrachloro-6-[[[3-[[(pentadecafluoroheptyl)sulfonyl]oxy]phenyl]amino]carbonyl]-, monopotassium salt |
| Synonyms | potassium 2,3,4,5-tetrachloro-6-[[[3-[[perfluoroheptane sulfonyl]oxy]phenyl]amino]carbony]benzoate |
| Structural Formula |  |
| Molecular Formula | $C_{21}H_5Cl_4F_{15}KNO_6S$ |
| Molecular Weight (g/mol) | 865.22 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)Oc1cc(NC(=O)c2c(C(=O)[O-])c(Cl)c(Cl)c(Cl)c2Cl)ccc1.[K+] |

The substance represented by CAS RN 68891-97-4 is a dinuclear coordination complex of chromium. The chromium ions in this complex are present in the 3+ oxidation state.

| | |
|---|---|
| CAS RN | 68891-97-4 |
| Chemical Name | Chromium, diaquatetrachloro[.mu.-[*N*-ethyl-*N*-[(pentadecafluoroheptyl)sulfonyl]glycinato-O1:O1']]-.mu.-hydroxybis(2-propanol)- |
| Synonyms | *N*-ethylperfluoroheptanesulfonylamido acetate chromium complex |
| Structural Formula |  |
| Molecular Formula | $C_{17}H_{28}Cl_4Cr_2F_{15}NO_9S$ |
| Molecular Weight (g/mol) | 953.25 |
| SMILES | C(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)N(CC1O[Cr+++]([OH]C(C)C)([OH2])([Cl-])([Cl-])[OH-][Cr+++]([OH2])([OH]C(C)C)([Cl-])([Cl-])O=1)CC |

## Physical and Chemical Properties

No experimental physical and chemical property data were located for the chemicals in this group.

The chemicals in this group include moderate to high molecular weight neutral organic chemicals, organic salts, and coordination complexes. The higher molecular weight chemicals, including the polyglycol derivatives, and chromium coordination complexes, are all expected to be involatile. However, the lower molecular weight neutral sulfonamides in this group may have some volatility. For example, the $C_4$ analogue chemical, *N*-MeFBSE acrylate (CAS RN 67584-55-8), has a reported vapour pressure of 0.25 Pa (ECHA, 2015c).

## Import, Manufacture and Use

## Australia

No specific Australian use, import, or manufacturing information has been identified. However, general information on the use of perfluoroalkyl sulfonates has been reported. The most recent data collected by NICNAS indicate that perfluoroalkyl sulfonates are predominantly used in Australia in mist suppressants for the metal plating industry and in fire fighting foams. Approximately 60 tonnes of fire fighting foams containing perfluoroalkyl sulfonates at concentrations up to 5% were held in Australia in 2007. Other uses included carpet treatments, curatives, industrial coatings and printing inks (NICNAS, 2013).

In 2004, it was reported that 1.6 tonnes of perfluoroalkyl sulfonates and related chemicals were imported into Australia. By 2007, the imported quantity of these chemicals had increased to 13.6 tonnes. It was reported that the majority of these imports were of chemicals based on the $C_4$ homologue, perfluorobutanesulfonic acid. The chemicals in this group are not manufactured in Australia (NICNAS, 2013).

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

## International

Due to their unique chemical properties perfluorinated chemicals and their precursors have found use in a wide range of industrial applications. However, concerns regarding the persistence and bioaccumulation hazards of long-chain perfluoroalkyl sulfonates resulted in the largest manufacturer of these chemicals ceasing their production in 2002 (Buck, et al., 2011). This is expected to have significantly reduced global supply of $C_6$ and $C_7$ perfluoroalkyl sulfonate derivatives. It should be noted, however, that perfluorohexanesulfonyl fluoride (CAS RN 423-50-7) is a likely precursor for many of the chemicals in this group and this chemical was reportedly produced in the United States in 2008 (OECD, 2011). Current production volumes of $C_5$ perfluoroalkyl sulfonate derivatives are unclear.

Nevertheless, many perfluoroalkyl sulfonamides and their derivatives appear to be used in the production of other fluorochemical products, such as surfactant materials (Buck, et al., 2011). The *N*-alkyl perfluoroalkanesulfonamide acrylates, such as CAS RNs 59071-10-2, 1893-52-3 and 68298-06-6, are reported to be used as co-monomers in the synthesis of acrylic polymers that are used in surface protection applications (Buck, et al., 2011).

In addition, use of the three perfluoroalkyl sulphonamide acetate salts in this group (CAS RNs 67584-52-5, 67584-53-6 and 67584-62-7) was reported in 2012 in Denmark (Nordic Council of Ministers, 2015). Data available for the homologous $C_8$ perfluoroalkyl sulphonamide acetate salt suggest these chemicals may have use in surface treatments, cleaning products and floor waxes (NICNAS, 2015c).

Less information is available for the remaining chemicals in this group. However, it is noted that data for the homologous $C_8$ chemicals suggest the perfluoroalkyl sulfonamide phosphate esters may be used in fabric paper treatments, paints, lacquers and varnishes, while the polyglycol derivatives may be used in surfactant preparations (NICNAS, 2015c).

# Environmental Regulatory Status

## Australia

In 2008, a factsheet published by NICNAS recommended that PFOS-based and related PFAS-based chemicals be restricted to essential uses only, and that importers ensure that alternative chemicals are less toxic and not persistent in the environment (NICNAS, 2013).

## 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, 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 having perfluoroheptyl derivatives with the formula $C_7F_{15}$ as a structural element, except those derivatives with the formula $C_7F_{15}$-X, where X = F, Cl, Br are listed under Schedule 1 (the Toxic Substances List) of the *Canadian Environmental Protection Act 1999* (Government of Canada, 1999). A proposal to prohibit the import, manufacture and use of these chemicals has been released, and is expected to be finalised by January 2016 (Environment Canada, 2012).

The majority of the chemicals in this group are listed on the Canadian Domestic Substances List (DSL) (Environment Canada, 2013). Of the 32 chemicals that are listed, 6 chemicals (CAS RNs 34455-03-3, 67940-02-7, 68555-72-6, 68555-73-7, 68555-75-9 and 68555-76-0) were found to be Persistent (P), Bioaccumulative (B) and Inherently Toxic to the Environment ($iT_E$) during the categorization of the DSL. With one exception, all of the chemicals listed were found to be P. While half the listed chemicals are found to be not B, the majority of the listed chemicals are $iT_E$.

## European Union

Sixteen chemicals in this group are currently subject to a restriction proposal to ban their manufacture, use, and placing on the market, either as substances on their own, as constituents of other substances, in a mixture or in articles. The chemicals under consideration are substances having a linear or branched perfluoroheptyl derivatives with the formula $C_7F_{15}$ as a structural element, including its salts except those derivatives with the formula $C_7F_{15}$-X, where X= F, Cl, Br (ECHA, 2015b).

Thirty six chemicals in this group have been pre-registered for use in the European Union under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation (ECHA, 2015a), but no chemicals in this group have undergone the full registration process (ECHA, 2015c).

## United States of America

Most of the chemicals in this group (40 substances, which includes perfluorinated chain lengths between $C_5$ and $C_7$) 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, 2014). These chemicals are subject to a Significant New Use Rule (SNUR). Any new uses, as defined under the rule, require approval from the United States Environmental Protection Agency (US EPA) (United States Government, 2002; 2007). The US EPA is currently proposing to modify this SNUR to make inapplicable the exemption for persons who import these substances as a component of carpets (US EPA, 2015).

The US EPA published an action plan on long-chain perfluorinated chemicals in 2009 due to their persistent, bioaccumulative and toxic hazard characteristics. The action plan includes the chemicals in this group with chains of six and seven perfluorinated carbons (US EPA, 2009).

# Environmental Exposure

Use of most chemicals in this group is expected to have been significantly phased out due to international concerns regarding the persistence and bioaccumulation hazards of long-chain perfluoroalkyl sulfonates (Buck, et al., 2011). The limited domestic

and international use data available suggest that current industrial uses are likely specialist and low volume in nature. Therefore, significant use of these chemicals in Australia is not expected, and widespread direct release of the chemicals in this group to the environment as a result of current industrial uses is considered unlikely.

The environmental degradants of primary concern for the chemicals of this group are the $C_5$ to $C_7$ perfluoroalkyl sulfonate anions. These perfluorinated anions are highly resistant to degradation in the environment. In addition, PFHxS and PFHpS have been found to be bioaccumulative, and PFPeS may be bioaccumulative, although the magnitude of the bioaccumulation hazard is currently uncertain (NICNAS, 2015b).

Biodegradation data available for the $C_8$*N*-ethylperfluorooctanesulfonamidoethyl alcohol (CAS RN 1691-99-2) demonstrate conversion to a carboxylic acid, with the ultimate biodegradation product being PFOS (Hekster, et al., 2002; Martin, et al., 2010). Other chemicals containing the perfluorooctyl sulfonate group are expected to be susceptible to a similar biotransformation process (Martin, et al., 2010). Further, data available for the $C_4$*N*-methylperfluorobutanesulfonamidoethyl alcohol (CAS RN 34454-97-2) indicate potential for atmospheric degradation to PFBS through oxidation by hydroxyl radicals (D'eon, et al., 2006; Martin, et al., 2010). Based on the results of these studies, the chemicals in this group are also expected to have potential to degrade to their respective perfluoroalkyl sulfonate anions in the environment.

Limited environmental monitoring data are available for the chemicals in this group or their expected intermediate degradation products. It has previously been suggested that this may be due to the lack of available reference standards (Schultz, et al., 2004). Nevertheless, the final perfluoroalkyl sulfonate degradation products have been detected in the environment. In particular, PFHxS has been widely detected (NICNAS, 2015b). This perfluoroalkyl sulfonate has been detected in the Parramatta and Brisbane river catchments in Australia at concentrations up to 17 nanograms per litre (ng/L) (Gallen, et al., 2014; Thompson, et al., 2011). However, it is noted there are multiple potential sources of perfluoroalkyl sulfonates in the environment, including past industrial use of direct precursors to perfluoroalkyl sulfonates or use of perfluoroalkyl sulfonate-related substances in articles, in addition to the industrial use of the chemicals in this group which may degrade to these perfluorinated anions in the environment.

## Environmental Effects

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

The currently available ecotoxicity data for $C_5$ to $C_7$ perfluoroalkyl sulfonates are summarised in the IMAP Environment Tier II assessment of Direct Precursors for Direct Precursors of Perfluoroheptanesulfonate (PFHpS), Perfluorohexanesulfonate (PFHxS) and Perfluoropentanesulfonate (PFPeS) (NICNAS, 2015b). Limited data are available for these direct precursors. However, it was concluded that $C_5$ to $C_7$ perfluoroalkyl sulfonates may have long-term toxic effects in aquatic organisms based on data which demonstrate that the $C_8$ homologue can cause chronic intergenerational toxicity in fish (NICNAS, 2015b).

It is noted that the chemicals in this group contain a range of functional groups and moieties which are correlated with acute toxic effects in aquatic organisms. However, these possible effects have not been considered in this assessment, as the primary risk posed by the chemicals in this group is assumed to result from the cumulative release of $C_5$ to $C_7$ perfluoroalkyl sulfonates into the environment.

## Categorisation of Environmental Hazard

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

It is noted that direct precursors of PFHpS and PFHxS are categorised as persistent (P) and bioaccumulative (B) substances according to domestic environmental hazard criteria. Direct precursors to PFPeS are categorised as persistent (P), but the bioaccumulation categorisation is uncertain (Uncertain B). In addition, the toxicity categorisation of all direct precursors to these perfluorinated anions is uncertain (Uncertain T) (NICNAS, 2015b).

## Risk Characterisation

The chemicals in this group have the potential to breakdown into persistent perfluoroalkyl sulfonates, which are known to be, or may be, bioaccumulative.

Chemicals which are persistent and bioaccumulative remain in the environment and accumulate in biota over an extended period of time, even if new emissions of the chemicals cease. These characteristics can result in very high internal concentrations in exposed organisms, which may cause long-term toxic effects that are not readily identified through standard testing protocols. Chemicals with these hazard characteristics are therefore considered to be of concern for the environment.

The bioaccumulation potential of PFPeS is uncertain. However, the high bioaccumulation potential of its immediate homologue, PFHxS, and the consistent detection of PFPeS in biota suggest that the $C_5$ homologue should also be considered of concern for the environment (NICNAS, 2015b).

## Key Findings

Chemicals in this group are expected to have been largely phased out of use due to international concerns about the persistence and bioaccumulation hazards of long-chain perfluoroalkyl sulfonates.

The principal risk posed by the chemicals in this group if emitted to the environment has been assumed to result from the cumulative release of $C_5$ to $C_7$ perfluoroalkyl sulfonate anions as breakdown products of the parent substances in this group. These perfluorinated anions are extremely persistent in the environment and are, or may be, bioaccumulative. The persistence and bioaccumulation potential of these anions increases the potential for chronic toxicity. The very persistent and very bioaccumulative $C_8$ perfluoroalkyl sulfonate anion (PFOS) can cause chronic intergenerational toxicity in fish. However, no chronic toxicity data are available for the homologous $C_5$ to $C_7$ sulfonates.

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

The assessment of the risks from these chemicals to human health, including public health, has been considered in the IMAP Human Health Tier II assessment for Indirect Precursors of Perfluoroalkane Sulfonic Acids (C5-C7) (NICNAS, 2015f).

## Recommendations

The chemicals in this group have been assessed as having the potential to give rise to adverse outcomes for the environment and public health. These chemicals are currently listed on the Australian Inventory of Chemical Substances (the Inventory), and are available to be introduced into Australia without 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 PFHpS, PFHxS and PFPeS have been classified as Chronic Aquatic Category 4 (H413: May cause long lasting harmful effects to aquatic life) under the GHS (NICNAS, 2015b).

## References

Buck RC, Franklin J, Berger U, Conder JM, Cousins IT, de Voogt P, Jensen AA, Kannan K, Mabury SA and van Leeuwen SP (2011). Perfluoroalkyl and Polyfluoroalkyl Substances in the Environment: Terminology, Classification and Origins. *Integrated Environmental Assessment and Management,* **7**(4), pp 513-541.

D'eon JC, Hurley MD, Wallington TJ and Mabury SA (2006). Atmospheric Chemistry of N-methyl Perfluorobutane Sulfonamidoethanol, $C_4F_9CO_2N(CH_3)CH_2CH_2OH$: Kinetics and Mechanism of Reaction with OH. *Environmental Science and Technology,* **40**(6), pp 1862-1868.

ECHA (2015a). *Pre-registered substances*. European Chemicals Agency, Helsinki, Finland. Accessed 1 April 2015 at http://echa.europa.eu.

ECHA (2015b). *Restrictions under consideration*. European Chemicals Agency, Germany. Accessed 19 June 2015 at http://echa.europa.eu.

ECHA (2015c). *Registered Substances Database*. European Chemicals Agency, Helsinki, Finland. Accessed 1 April 2015 at http://echa.europa.eu.

Environment Canada (2012). *Proposed Risk Management Approach for Perfluorooctanoic Acid (PFOA), its Salts, and its Precursors and Long-Chain (C9-C20) Perfluorocarboxylic Acids (PFCAs), their Salts, and their Precursors*. Environment Canada, Gatineau, Canada. Accessed 25 February 2015 at http://www.ec.gc.ca.

Environment Canada (2013). *Search Engine for Substances on the DSL, Government Canada results for all Existing Substances*. Environment Canada, Gatineau, Quebec, Canada. Accessed 7 November 2013 http://www.ec.gc.ca.

EPHC (2009). *Environmental Risk Assessment Guidance Manual for Industrial Chemicals*. Environment Protection and Heritage Council, Canberra, Australia. Accessed 9 December 2013 at http://www.scew.gov.au.

Gallen C, Baduel C, Lai FY, Thompson K, Thompson J, Warne M and Mueller J (2014). Spatio-temporal assessment of perfluorinated compounds in the Brisbane River system, Australia: Impact of a major flood event. *Marine Pollution Bulletin,* **85**, pp 597-605.

Government of Canada (1999). *Canadian Environmental Protection Act, 1999*. Accessed 19 June 2015 at http://laws-lois.justice.gc.ca.

Hekster F, de Voogt P, Pijnenburg A and Laane R (2002). *Perfluoroalkylated substances: Aquatic environmental assessment, Report RIKZ/2002.043*. Government of the Netherlands Ministry of Infrastructure and the Environment, Amsterdam, The Netherlands. Accessed 22 December 2014 at http://repository.tudelft.nl.

Martin JW, Asher BJ, Beesoon S, Benskin JP and Ross MS (2010). PFOS or PreFOS? Are perfluorooctane sulfonate precursors (PreFOS) important determinants of human and environmental perfluorooctane sulfonate (PFOS) exposure? *Journal of Environmental Monitoring,* **12**(11), pp 1979-2004.

NICNAS (2013). *PFC Derivatives and Chemicals on which they are based: Alert Factsheet*. National Industrial Chemicals Notification and Assessment Scheme, Sydney, Australia. Accessed 11 November 2014 at http://www.nicnas.gov.au.

NICNAS (2015a). *IMAP Environment Tier II Assessment for Direct Precursors to Perfluorooctanesulfonate (PFOS)*. National Industrial Chemicals Notification and Assessment Scheme, Sydney, Australia.

NICNAS (2015b). *IMAP Environment Tier II Assessment for Direct Precursors to Perfluoroheptanesulfonate (PFHpS), Perfluorohexanesulfonate (PFHxS) and Perfluoropentanesulfonate (PFPeS)*. National Industrial Chemicals Notification and Assessment Scheme, Sydney, Australia.

NICNAS (2015c). *Environment Tier II Assessment for Indirect Precursors to Perfluorooctanesulfonate (PFOS)*. National Industrial Chemicals Notification and Assessment Scheme, Sydney, Australia. http://www.nicnas.gov.au.

NICNAS (2015d). *NICNAS Handbook for Notifiers*. National Industrial Chemicals Notification and Assessment Scheme, Sydney, Australia. Accessed 28 January 2015 at http://www.nicnas.gov.au.

NICNAS (2015e). *IMAP Environment Tier II Assessment for Perfluorobutanesulfonic Acid and its Direct Precursors*. National Industrial Chemicals Notification and Assessment Scheme, Sydney, Australia.

NICNAS (2015f). *IMAP Human Health Tier II assessment for Indirect Precursors of Perfluoroalkane Sulfonic Acids (PFSA) (C5-C7)* National Industrial Chemicals Notification and Assessment Scheme, Sydney, Australia.

Nordic Council of Ministers (2015). *Substances in Preparations in Nordic Countries (SPIN)*. Chemical Group, Nordic Council of Ministers, Copenhagen, Denmark. Accessed 17 March 2015 at http://www.spin2000.net.

OECD (2011). *PFCS: Outcome of the 2009 Survey on the Production, Use and Release of PFOS, PFAS, PFOA, PFCA, Their Related Substances and Products/Mixtures Containing These Substances*. Organisation for Economic Cooperation and Development, Paris, France. Accessed 9 January 2015 at http://www.oecd.org.

OECD (2013). *OECD Existing Chemicals Database*. Organisation for Economic Cooperation and Development, Paris, France. Accessed 13 November 2013 http://webnet.oecd.org.

Schultz M, Barofsky D and Field J (2004). Quantitative Determination of Fluorotelomer Sulfonates in Groundwater by LC MS/MS. *Environmental Science and Technology* **38**(6), pp 1828-1835.

Thompson J, Roach A, Eaglesham G, Bartkow ME, Edge K and Mueller J (2011). Perfluorinated alkyl acids in water, sediment and wildlife from Sydney Harbour and surroundings. *Marine Pollution Bulletin,* **62**, pp 2869-2875.

UNECE (2009). *Globally Harmonised System of Classification and Labelling of Chemicals (GHS), 3rd Revised Edition*. United Nations Economic Commission for Europe, Geneva, Switzerland. Accessed 12 November 2013 at http://www.unece.org

UNEP (1987). *The Montreal Protocol on Substances that Deplete the Ozone Layer*. United Nations Environment Programme, Ozone Secretariat, Nairobi, Kenya. Accessed 12 November 2013 at http://ozone.unep.org.

UNEP (2001). *The Stockholm Convention on Persistent Organic Pollutants*. United Nations Environment Programme, Secretariat of the Stockholm Convention, Châtelaine, Switzerland. Accessed 12 November 2013 at http://www.pops.int.

UNEP & FAO (1998). *The Rotterdam Convention on the Prior Informed Consent procedure for Certain Hazardous Chemicals and Pesticides in International Trade*. United Nations Environment Programme and Food and Agriculture Organization of the United Nations, Châtelaine, Switzerland. Accessed 12 November 2013 at http://www.pic.int.

United States Government (2002). Perfluoroalkyl Sulfonates; Significant New Use Rule. *Federal Register,* **67**(236), pp 72854-72867.

United States Government (2007). Perfluoroalkyl Sulfonates; Significant New Use Rule. *Federal Register,* **72**(194), pp 57222-57235.

US EPA (2009). *Long-Chain Perfluorinated Chemicals (PFCs) Action Plan*. United States Environmental Protection Agency, Washington DC, USA. Accessed 10 December 2014 at http://www.epa.gov.

US EPA (2014). *TSCA Chemical Substance Inventory*. United States Environmental Protection Agency, Washington DC, USA. Accessed 26 February 2015 at http://www.epa.gov.

US EPA (2015). *Significant New Use Rules: Long-Chain Perfluoroalkyl Carboxylate and Perfluoroalkyl Sulfonate Chemical Substances*. United States Environmental Protection Agency, Washington DC, USA. Accessed 25 February 2015 at http://www.regulations.gov.

*Last update 3 July 2015*

Share this page