

What is a PFAS?..and the challenges associated with defining them

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The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA

ORIGINAL RESEARCH article

Front. Environ. Sci., 05 April 2022

Sec. Toxicology, Pollution and the
Environment

<https://doi.org/10.3389/fenvs.2022.850019>

This article is part of the Research Topic

Environmental Pollution and Toxicity of Emerging Per- and Polyfluoroalkyl
Substances (PFASs)

[View all Articles >](#)

Assembly and Curation of Lists of Per- and Polyfluoroalkyl Substances (PFAS) to Support Environmental Science Research



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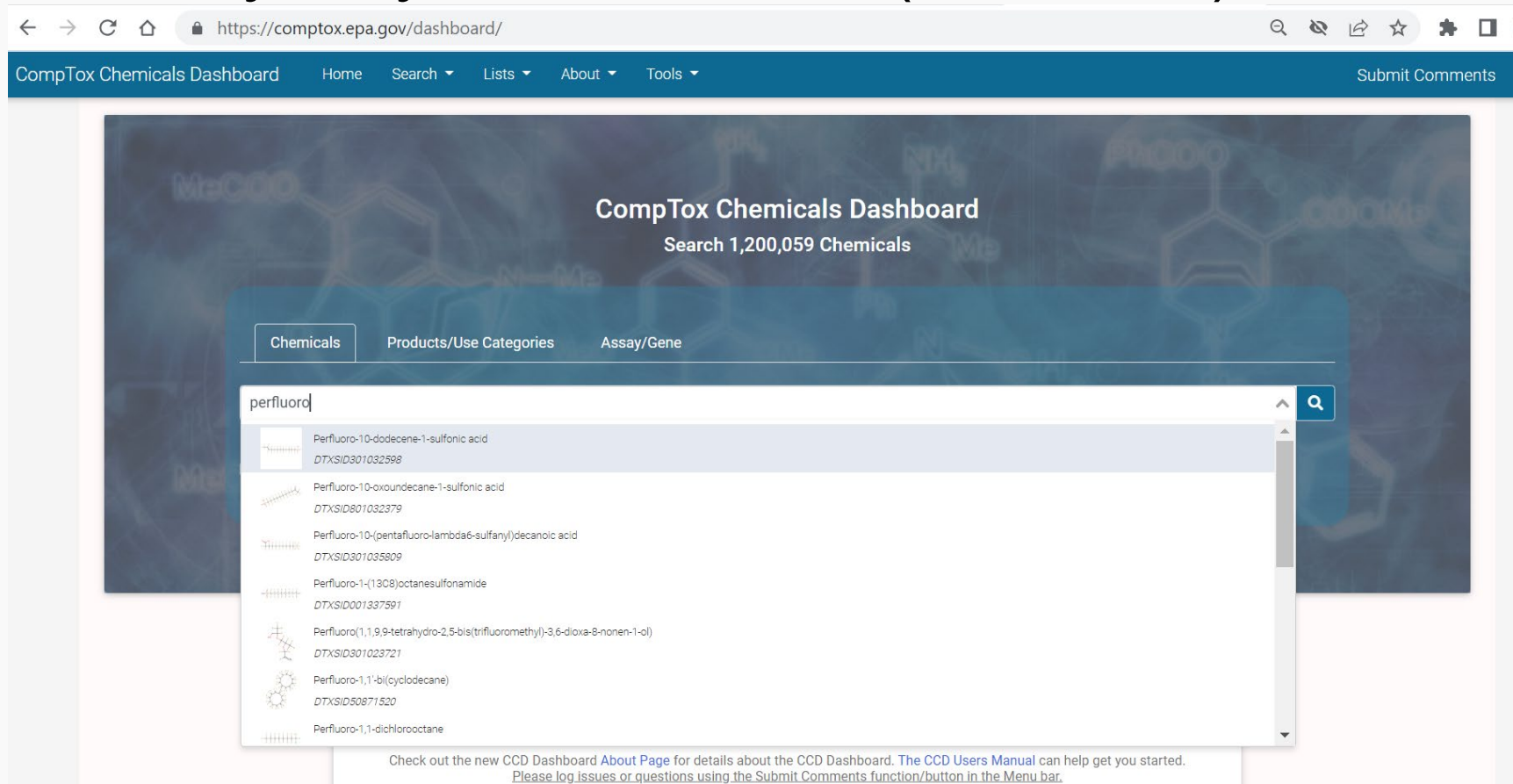
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- **A publicly accessible website** delivering access to:
 - ~1.2M chemicals with related property data
 - Experimental and predicted physicochemical property data
 - Experimental Human and Ecological hazard data
 - Integration to “biological assay data” for 1000s of chemicals
 - Information regarding chemicals in consumer products
 - Links to other agency websites and public data resources
 - “Literature” search capability for chemicals using public resources
 - “Batch searching” for tens to thousands of chemicals
- **Over 15,000 of the chemicals are classed as PFAS Chemicals (but be cautious regarding the definition of a PFAS”...)**

CompTox Chemicals Dashboard

<https://comptox.epa.gov/dashboard>

- Searching – CAS Numbers, systematic names and synonyms, structures (as InChIs)



The screenshot shows the CompTox Chemicals Dashboard search interface. The browser address bar displays <https://comptox.epa.gov/dashboard/>. The dashboard header includes navigation links: Home, Search, Lists, About, and Tools, along with a "Submit Comments" button. The main content area features the title "CompTox Chemicals Dashboard" and the text "Search 1,200,059 Chemicals". Below this, there are tabs for "Chemicals", "Products/Use Categories", and "Assay/Gene". A search bar contains the text "perfluorol", and a dropdown menu displays a list of search results, each with a chemical structure icon, the full name, and the DTXSID. The results include:

- Perfluoro-10-dodecene-1-sulfonic acid (DTXSID301032598)
- Perfluoro-10-oxoundecane-1-sulfonic acid (DTXSID801032379)
- Perfluoro-10-(pentafluoro-lambda6-sulfanyl)decanoic acid (DTXSID301035809)
- Perfluoro-1-(13C8)octanesulfonamide (DTXSID001037591)
- Perfluoro(1,1,9,9-tetrahydro-2,5-bis(trifluoromethyl)-3,6-dioxo-8-nonen-1-yl) (DTXSID301023721)
- Perfluoro-1,1'-bi(cyclodecane) (DTXSID50871520)
- Perfluoro-1,1-dichlorooctane

At the bottom, a note states: "Check out the new CCD Dashboard [About Page](#) for details about the CCD Dashboard. [The CCD Users Manual](#) can help get you started. [Please log issues or questions using the Submit Comments function/button in the Menu bar.](#)"

Substring search “perfluoro”

- Substring search ~4665 chemicals. MANY perfluoro names added by our curators

Showing 4665 of 4665 chemicals

<p>N-Ethylperfluoro-1-dodeca... DTXSID : DTXSID401035521 CASRN : NOCAS_1035521 TOXCAST :</p>	<p>2H-Perfluoro-2-dodeceno... DTXSID : DTXSID70895723 CASRN : 70887-94-4 TOXCAST :</p>	<p>Bis(perfluoroethyl)fluorop... DTXSID : DTXSID901027038 CASRN : NOCAS_1027038 TOXCAST :</p>	<p>N-[3-(Dimethylamino)prop... DTXSID : DTXSID301032786 CASRN : 1513863-81-4 TOXCAST :</p>	<p>3-[(Perfluoropentanesulfo... DTXSID : DTXSID901033118 CASRN : 2089108-63-2 TOXCAST :</p>	<p>10-Chloro-perfluorodecan... DTXSID : DTXSID70892616 CASRN : 574715-86-9 TOXCAST :</p>
<p>Sodium perfluoro(3-[[1-(1,... DTXSID : DTXSID301032679 CASRN : 1383434-30-7 TOXCAST :</p>	<p>0 related chemical structures with this substance</p> <p>Fatty acids, C18-unsatd., ... DTXSID : DTXSID90881860 CASRN : 306974-63-0 TOXCAST :</p>	<p>Perfluoro-2-propyl 2H-per... DTXSID : DTXSID30479967 CASRN : 25352-92-5 TOXCAST :</p>	<p>Triethylaminium perfluoro... DTXSID : DTXSID30897521 CASRN : 165951-18-8 TOXCAST :</p>	<p>Bis(perfluoroethanesulfon... DTXSID : DTXSID20889011 CASRN : 152894-10-5 TOXCAST :</p>	<p>9-Chloro-perfluorononanoi... DTXSID : DTXSID30382104 CASRN : 865-79-2 TOXCAST : 157/514</p>

Substring search “perfluoro” “Explicit” structures

- >350 do not have explicit structures...

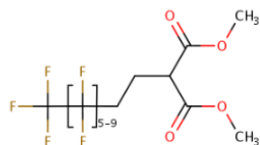
Showing 352 of 4665 chemicals
Filtering out chemicals that are: **Are Structures**

0 related chemical structures with this substance Bicyclo[2.2.1]heptane-2,3-... DTXSID : DTXSID50883087 CASRN : 71608-43-0 TOXCAST :	2 related chemical structures with this substance Copolymer of fluoroethen... DTXSID : DTXSID90880373 CASRN : 25120-57-4 TOXCAST :	0 related chemical structures with this substance Alcohols, C8-14, γ-ω-perfl... DTXSID : DTXSID20882648 CASRN : 223586-53-6 TOXCAST :	0 related chemical structures with this substance Perfluoropentane sulfinic ... DTXSID : DTXSID701033100 CASRN : 1997344-06-5 TOXCAST :	0 related chemical structures with this substance Perfluoro-(C6-18)-alkylpho... DTXSID : DTXSID001021283 CASRN : NOCAS_1021283 TOXCAST :	0 related chemical structures with this substance Sulfonamides, C4-8-alkan... DTXSID : DTXSID00883077 CASRN : 192662-29-6 TOXCAST :
0 related chemical structures with this substance Thiols, C4-20, .gamma.-o... DTXSID : DTXSID40882988 CASRN : 151686-30-5 TOXCAST :	3 related chemical structures with this substance Propanedioic acid, mono(... DTXSID : DTXSID40883071 CASRN : 238420-90-9 TOXCAST :	0 related chemical structures with this substance Poly-1,1-difluoroethene-co... DTXSID : DTXSID70881904 CASRN : 355015-68-8 TOXCAST :	0 related chemical structures with this substance 11-(Perfluorododecyl)-3,6... DTXSID : DTXSID801339389 CASRN : NOCAS_1339389 TOXCAST :	2 related chemical structures with this substance Thiols, C8-20, gamma-om... DTXSID : DTXSID10881943 CASRN : 70969-47-0 TOXCAST :	0 related chemical structures with this substance 2-Propenoic acid, .gamma... DTXSID : DTXSID40882781 CASRN : 221455-61-4 TOXCAST :
0 related chemical structures	0 related chemical structures	0 related chemical structures	0 related chemical structures	2 related chemical structures	0 related chemical structures

↑

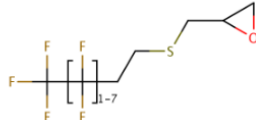
Substring search “perfluoro” “Markush” representations

- As of August 2022, there are 328/1340 PFAS Markush representations out of the whole DB



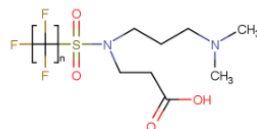
Propanedioic acid, mono(...

DTXSID : DTXSID20881893
CASRN : 238420-68-3
TOXCAST :



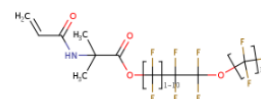
Oxirane, 2-((gamma-ome...

DTXSID : DTXSID00881336
CASRN : 119438-11-8
TOXCAST :



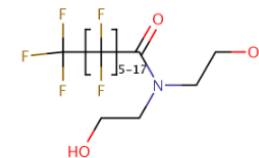
Perfluoroalkyl sulfonamid...

DTXSID : DTXSID10892978
CASRN : NOCAS_892978
TOXCAST :



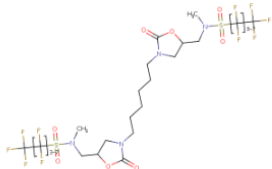
Alanine, 2-methyl-N-(1-oxo...

DTXSID : DTXSID30883060
CASRN : 161075-35-0
TOXCAST :



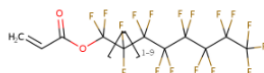
Perfluoroalkyl(C7-19)amid...

DTXSID : DTXSID30881309
CASRN : 90622-99-4
TOXCAST :



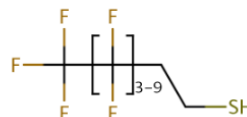
Sulfonamides, C4-8-alkan...

DTXSID : DTXSID10883023
CASRN : 306980-27-8
TOXCAST :



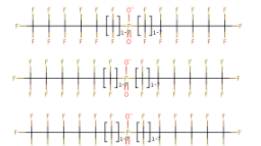
2-Propenoic acid, perfluor...

DTXSID : DTXSID20881292
CASRN : 85681-64-7
TOXCAST :



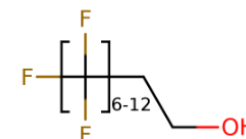
Perfluoroalkyl(C4-10)ethyl...

DTXSID : DTXSID30881905
CASRN : 68140-20-5
TOXCAST :



Phosphinic acid, bis(perfl...

DTXSID : DTXSID90881325
CASRN : 93062-53-4
TOXCAST :

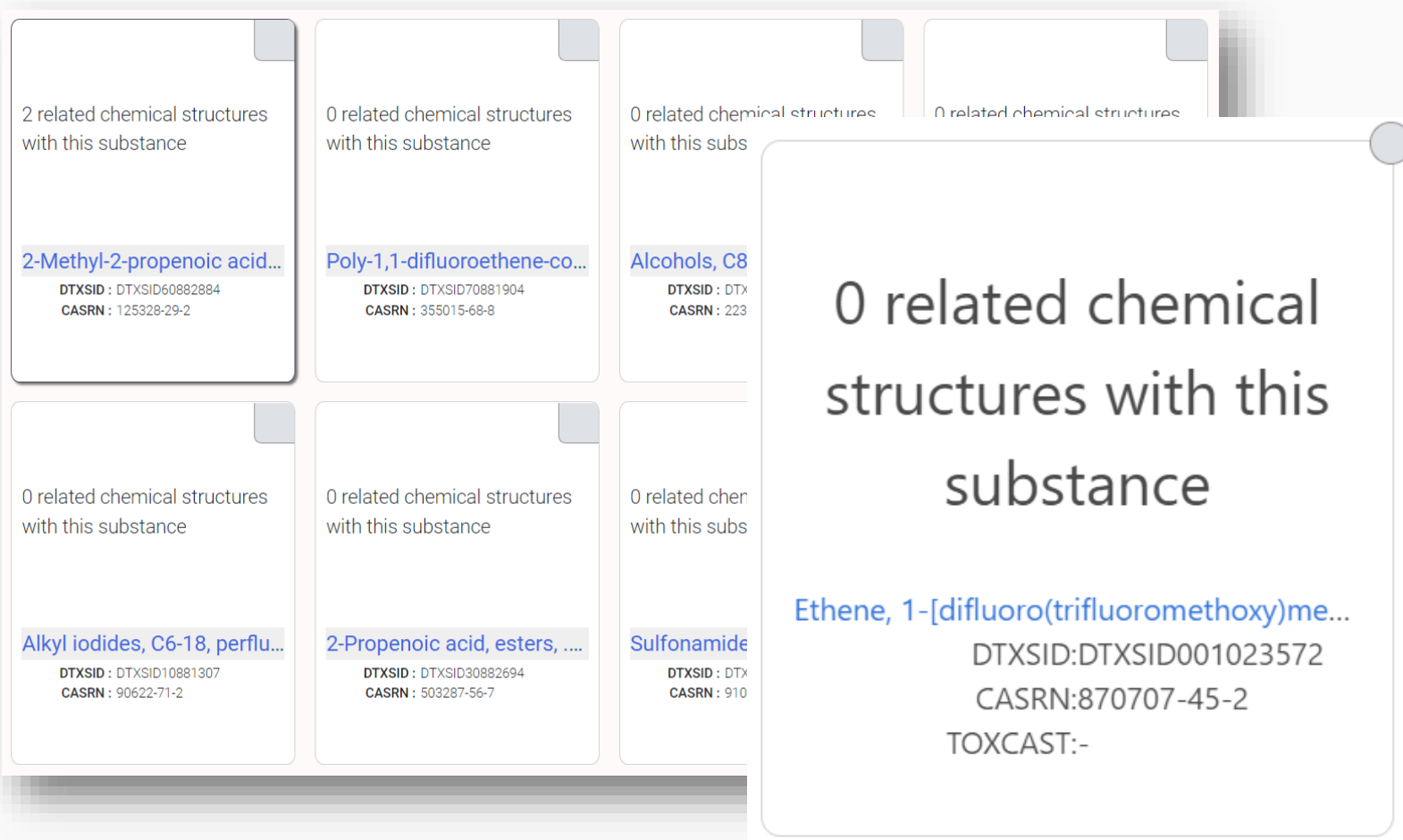


Alcohols, C8-14, .gamma-...

DTXSID : DTXSID70883049
CASRN : 68391-08-2
TOXCAST :

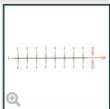
Substring search “perfluoro” “UVCB” chemicals

- Unknown or Variable Composition, Complex Reaction Products and Biological Materials



Chemical Name	DTXSID	CASRN	Related Structures
2-Methyl-2-propenoic acid...	DTXSID: DTXSID60882884	CASRN: 125328-29-2	2 related chemical structures with this substance
Poly-1,1-difluoroethene-co...	DTXSID: DTXSID70881904	CASRN: 355015-68-8	0 related chemical structures with this substance
Alcohols, C8	DTXSID: DTX	CASRN: 223	0 related chemical structures with this substance
Alkyl iodides, C6-18, perflu...	DTXSID: DTXSID10881307	CASRN: 90622-71-2	0 related chemical structures with this substance
2-Propenoic acid, esters, ...	DTXSID: DTXSID30882694	CASRN: 503287-56-7	0 related chemical structures with this substance
Sulfonamide	DTXSID: DTX	CASRN: 910	0 related chemical structures with this substance
Ethene, 1-[difluoro(trifluoromethoxy)me...	DTXSID: DTXSID001023572	CASRN: 870707-45-2	0 related chemical structures with this substance

CompTox Chemicals Dashboard
Home
Search
Lists
About
Tools
Submit Comments
Search all data



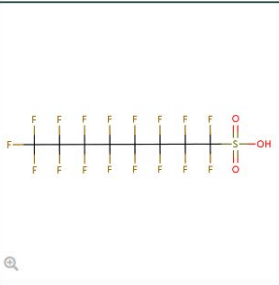
Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by DTXSID

Details
Executive Summary
Properties
Env. Fate/Transport
Hazard
Safety > GHS Data
ADME > IVIVE
Exposure
Bioactivity
Similar Compounds
GenRA
Related Substances
Synonyms
Literature
Links
Comments

Chemical Details



Wikipedia

Perfluorooctanesulfonic acid (PFOS) (conjugate base **perfluorooctanesulfonate**) is a chemical compound having an eight-carbon fluorocarbon chain and a sulfonic acid functional group and thus a perfluorosulfonic acid. It is an anthropogenic (man-made) fluorosurfactant, now regarded as a global pollutant. PFOS was the key ingredient in Scotchgard, a fabric protector made by 3M, and related stain repellents. The acronym "PFOS" refers to the parent sulfonic acid and to various salts

[Read more](#)

Quality Control Notes

Intrinsic Properties

Molecular Formula: C₈HF₁₇O₃S

MOL FILE
FIND ALL CHEMICALS

Average Mass: 500.13 g/mol

ISOTOPE MASS DISTRIBUTION

Monoisotopic Mass: 499.937494 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Physicochemical Properties

Properties: Summary

Summary



Search Chemical Properties

EXPORT

Summary

Property	experimental	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
LogKow: Octanol-Water	5.61 (3)	5.77 (4)	5.50	5.94	4.30 to 7.03	4.17 to 7.03	-
Vapor Pressure	2.48e-6 (1)	2.48e-6 (1)	2.48e-6	2.48e-6	2.48e-6	2.48e-6	mmHg
Boiling Point	169 (4)	231 (3)	148	229	133 to 249	219 to 244	°C
Water Solubility	1.14e-3 (2)	0.567 (4)	1.14e-3	4.11e-4	1.14e-3	6.25e-9 to 2.27	mol/L
Henry's Law	-	1.80e-11 (1)	-	1.80e-11	-	1.80e-11	atm-m3/mole
Polarizability	-	20.4 (1)	-	20.4	-	20.4	Å^3
Melting Point	-	84.1 (3)	-	51.9	-	15.2 to 185	°C
Molar Refractivity	-	51.5 (1)	-	51.5	-	51.5	cm^3
Molar Volume	-	272 (1)	-	272	-	272	cm^3
Surface Tension	-	19.6 (1)	-	19.6	-	19.6	dyn/cm
Density	-	1.84 (2)	-	1.84	-	1.84 to 1.85	g/cm^3
Index of Refraction	-	1.30 (1)	-	1.30	-	1.30	-
LogKoa: Octanol-Air	-	4.75 (1)	-	4.75	-	4.75	-

Experimental Data

Properties: LogKow: Octanol-Water

LogKow: Octanol-Water

Search Chemical Properties

EXPORT

Summary

Type	Average	Median	Range	Unit
Experimental	5.61	5.50	4.30 to 7.03	
Predicted	5.77	5.94	4.17 to 7.03	

EXPORT

Experimental

Source	Result	Experimental Details
Rayne et al, J. Env. Sci. and Health Part A, (2009) 44(12):1145-1199		Sierra Rayne & Kaya Forest (2009) Perfluoroalkyl sulfonic and carboxylic acids: A critical review of physicochemical properties, levels and patterns in waters and wastewaters, and treatment methods, Journal of Environmental Science and Health Part A, 44:12, 1145-1199, DOI: 10.1080/10934520903139811. (J. Env. Sci. and Health Part A, (2009) 44(12):1145-1199)
NCCT_Physchem		
NCCT_Physchem		

EXPORT

Predicted

Source	Result	Calculation Details	QMRF
ACD/Labs Consensus	4.17	Not Available	Not Available
OPERA	5.61	OPERA Calculation Report [Inside AD]	Available
EPISUITE	6.28	Not Available	Not Available

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Environmental Chemistry

Property Estimation of Per- and Polyfluoroalkyl Substances: A Comparative Assessment of Estimation Methods

Alina Lampic and J. Mark Parnis*

Chemical Properties Research Group (Canadian Environmental Modelling Centre), Department of Chemistry, Trent University, Peterborough, Ontario, Canada

- Comparison of COSMOtherm, EPI Suite ACD/Labs, TEST and OPERA
- OPERA **best performance**: Vapor Pressure, Solubility, Octanol-water partitioning, Octanol-Air partitioning, Soil-Adsorption coefficient

What is PFOS Called?

Synonyms, CASRN and more

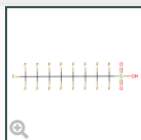
Synonyms

Search Chemical Synonyms		EXPORT
Synonym	Quality	
<input type="text"/>	<input type="text"/>	
1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-Heptadecafluoro-1-octanesulfonic acid	Valid	
1763-23-1 Active CAS-RN	Valid	
1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-	Valid	
1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-	Valid	
1-Octanesulfonic acid, heptadecafluoro-	Valid	
1-Perfluorooctanesulfonic acid	Valid	
heptadecafluoro-1-octanesulfonic acid	Valid	
heptadecafluorooctane-1-sulfonic acid	Valid	
Heptadecafluorooctane-1-sulfonic acid	Valid	
heptadecafluorooctane-1-sulphonic acid	Valid	
Heptadecafluorooctanesulfonic acid	Valid	
Perfluoro-n-octane 1-sulfonic acid	Valid	
perfluorooctane-1-sulfonic acid	Valid	
perfluorooctane sulfonic acid	Valid	
Perfluorooctanesulfonic acid	Valid	
Rows: 30		Total Rows: 30

- Similar compounds - based on structure “fingerprints”
- Structure mappings - between parent and salts, multicomponent chemicals, isotopomers
- Related substances – monomer to polymer, parent to transformation products

Are there Similar Compounds?

127 chemicals >0.8 match factor



Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by Synonym.

Searched with a similarity threshold of 0.8

Search Results SEND 127 TO BATCH SEARCH TILE INFO FILTER EXPORT PREFERRED VIEW

Showing 127 of 127 chemicals

Details

Executive Summary

Properties

Env. Fate/Transport

Hazard

Safety > GHS Data

ADME > IVIVE

Exposure

Bioactivity

Similar Compounds

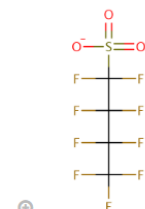
GenRA

Related Substances

Synonyms

Literature

Links



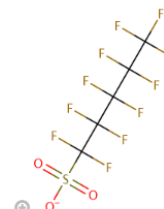
Perfluorobutanesulfonate

DTXSID : DTXSID60873015
CASRN : 45187-15-3
Similarity : 1.00



Perfluorobutanesulfonic a...

DTXSID : DTXSID5030030
CASRN : 375-73-5
Similarity : 1.00



Perfluoropentanesulfonate

DTXSID : DTXSID70892479
CASRN : 175905-36-9
Similarity : 1.00



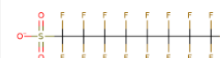
Perfluoropentanesulfonic ...

DTXSID : DTXSID8062600
CASRN : 2706-91-4
Similarity : 1.00



Perfluorohexanesulfonate

DTXSID : DTXSID80873012
CASRN : 108427-53-8
Similarity : 1.00



Relationships in the data

Env. Fate/Transport

Hazard

Safety > GHS Data

ADME > IVIVE

Exposure

Bioactivity

Similar Compounds

GenRA

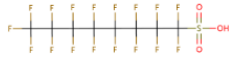
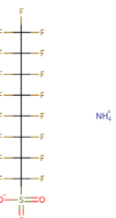

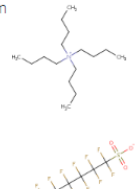
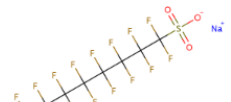
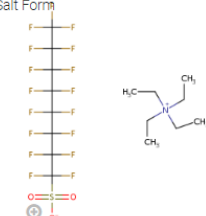


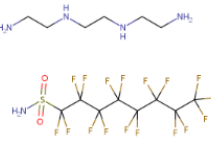

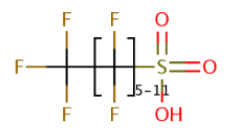
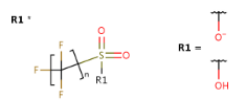
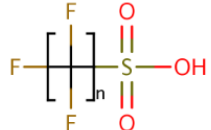
Related Substances

Synonyms

Literature

Links

Comments

<p>Searched Chemical</p>  <p>Perfluorooctanesulfonic a...</p> <p>DTXSID : DTXSID3031864 CASRN : 1763-23-1</p>	<p>Salt Form</p>  <p>Ammonium perfluoroocta...</p> <p>DTXSID : DTXSID9067435 CASRN : 29081-56-9</p>	<p>Salt Form</p>  <p>Lithium perfluorooctanes...</p> <p>DTXSID : DTXSID2032421 CASRN : 29457-72-5</p>	<p>Salt Form</p>  <p>Tetraethylammonium per...</p> <p>DTXSID : DTXSID40584995 CASRN : 111873-33-7</p>	<p>Salt Form</p>  <p>Sodium perfluorooctanes...</p> <p>DTXSID : DTXSID50635462 CASRN : 4021-47-0</p>
<p>Salt Form</p>  <p>Tetraethylammonium per...</p> <p>DTXSID : DTXSID5069128 CASRN : 56773-42-3</p>	<p>Salt Form</p>  <p>Potassium perfluoroocta...</p> <p>DTXSID : DTXSID8037706 CASRN : 2795-39-3</p>	<p>Salt Form</p>  <p>Magnesium perfluoroocta...</p> <p>DTXSID : DTXSID8081314 CASRN : 91036-71-4</p>	<p>Predecessor: Component</p>  <p>1-Octanesulfonic acid, 1,1,...</p> <p>DTXSID : DTXSID40880545 CASRN : 64202-77-3</p>	<p>Predecessor: Component</p> <p>3 related chemical structures with this substance</p> <p>Mixture of PFOS and PFOA</p> <p>DTXSID : DTXSID20872963 CASRN : NOCAS_872963</p>
<p>Component</p> 	<p>Markush Parent</p> 	<p>Markush Parent</p> 	<p>Markush Parent</p> 	

LISTS OF PFAS SUBSTANCES

PFAS Lists of Chemicals (45/416)

https://comptox.epa.gov/dashboard/chemical_lists

Q

Search Chemical Lists

EXPORT

COPY URL

Showing 45 of 416 Records

List Acronym

PFAS

CCL5PFAS

EPAPFAS75S1

Rows: 45 of 416

PFAS|EPA|WATER: PFAS with Validated EPA Drinking Water Methods

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey

☐ Identifier substring search

List Details

Description: List of PFAS for which a Standard Drinking Water method (537.1 or 533) exists and which will potentially to be included in UCMR5 (2023-2025)

Number of Chemicals: 31

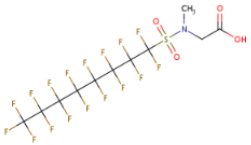
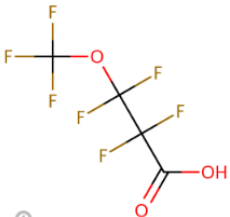



Search Results

SEND 31 TO BATCH SEARCH

TILE INFO

FILTER

Showing 31 of 31 chemicals

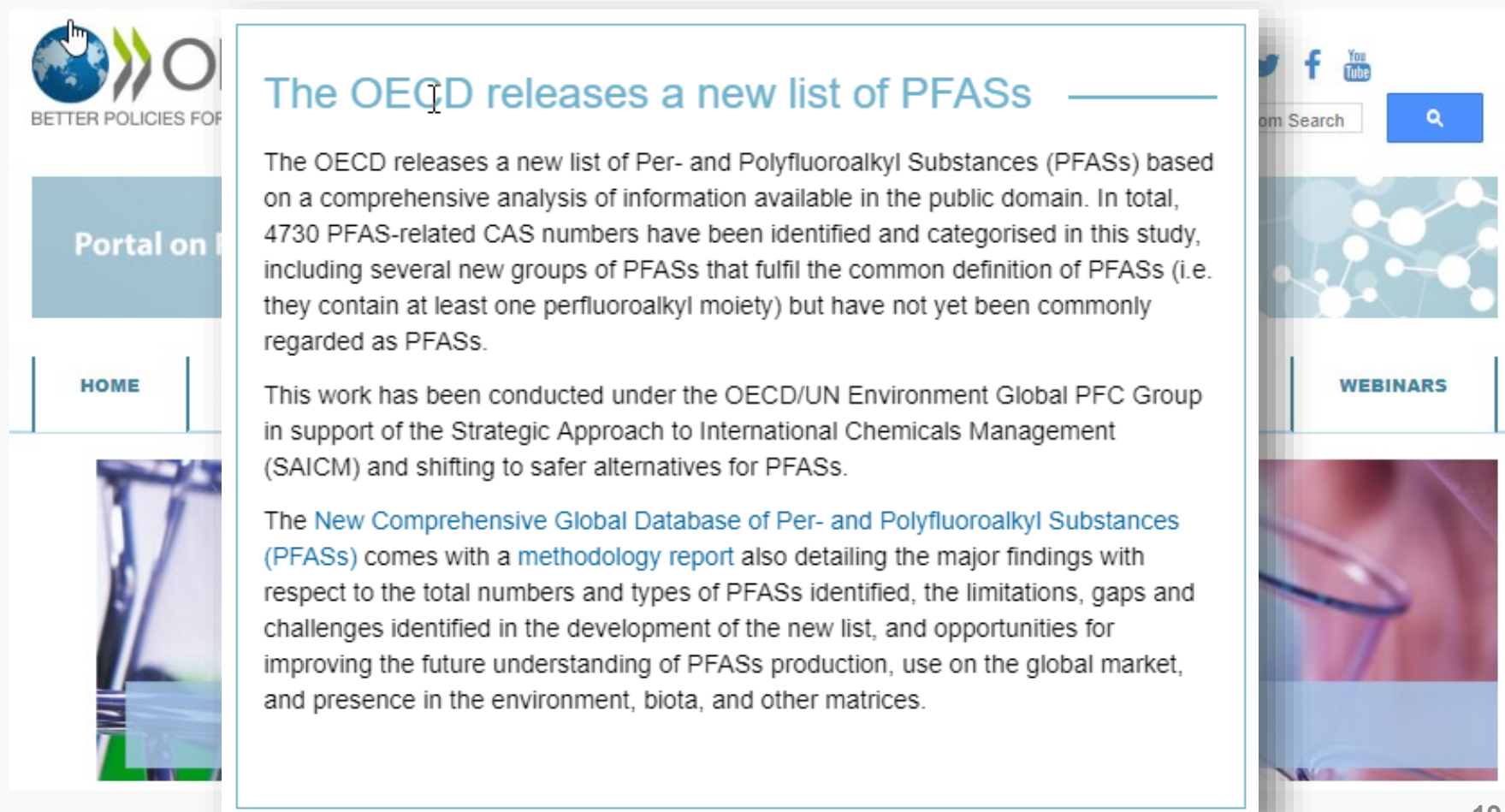


- Assembled chemical lists give access to curated data
 - Names and synonyms
 - Physicochemical/Fate and Transport data
 - Toxicity data
 - Relationships in the data
 - Regulatory lists

The OECD List of PFAS

<http://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals/>

- Most of this list did NOT have structures!!!



The screenshot shows the OECD Portal on PFAS. The header includes the OECD logo and the text "BETTER POLICIES FOR". The main content area is titled "The OECD releases a new list of PFASs". Below the title, there is a paragraph stating: "The OECD releases a new list of Per- and Polyfluoroalkyl Substances (PFASs) based on a comprehensive analysis of information available in the public domain. In total, 4730 PFAS-related CAS numbers have been identified and categorised in this study, including several new groups of PFASs that fulfil the common definition of PFASs (i.e. they contain at least one perfluoroalkyl moiety) but have not yet been commonly regarded as PFASs." This is followed by another paragraph: "This work has been conducted under the OECD/UN Environment Global PFC Group in support of the Strategic Approach to International Chemicals Management (SAICM) and shifting to safer alternatives for PFASs." The final paragraph states: "The [New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances \(PFASs\)](#) comes with a [methodology report](#) also detailing the major findings with respect to the total numbers and types of PFASs identified, the limitations, gaps and challenges identified in the development of the new list, and opportunities for improving the future understanding of PFASs production, use on the global market, and presence in the environment, biota, and other matrices." The sidebar on the right includes social media icons for Twitter, Facebook, and YouTube, a search bar, and a "WEBINARS" section.

The OECD releases a new list of PFASs

The OECD releases a new list of Per- and Polyfluoroalkyl Substances (PFASs) based on a comprehensive analysis of information available in the public domain. In total, 4730 PFAS-related CAS numbers have been identified and categorised in this study, including several new groups of PFASs that fulfil the common definition of PFASs (i.e. they contain at least one perfluoroalkyl moiety) but have not yet been commonly regarded as PFASs.

This work has been conducted under the OECD/UN Environment Global PFC Group in support of the Strategic Approach to International Chemicals Management (SAICM) and shifting to safer alternatives for PFASs.

The [New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances \(PFASs\)](#) comes with a [methodology report](#) also detailing the major findings with respect to the total numbers and types of PFASs identified, the limitations, gaps and challenges identified in the development of the new list, and opportunities for improving the future understanding of PFASs production, use on the global market, and presence in the environment, biota, and other matrices.

The OECD List of PFAS

<http://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals/>

List Details

Description: OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances (PFASs) listing more than 4700 new PFAS, including several new groups of PFASs that fulfill the common definition of PFASs (i.e. they contain at least one perfluoroalkyl moiety) but have not yet been commonly regarded as PFASs. The list can be used in conjunction with the methodology report summarising the major findings with respect to the total numbers and types of PFASs identified, the limitations, gaps and challenges identified, and opportunities for improving the future understanding of PFASs production, use on the global market, and presence in the environment, biota, and other matrices.

Source website: <http://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals>

A major effort was undertaken to register this list within DSSTox, adding chemical structures for as many PFAS entries as possible using both manual and auto-mapping (structures using CAS-matching) curation methods. The result is that approximately 1/3 of the list is curated at the highest two curation levels (DSSTox_High or DSSTox_Low) currently, whereas more than half of this list is registered at the Public_Low curation level (based on PubChem content). The PFASOECD list is undergoing continuous registration and curation.

Number of Chemicals: 4729

Search Results

SEND 4729 TO BATCH SEARCH

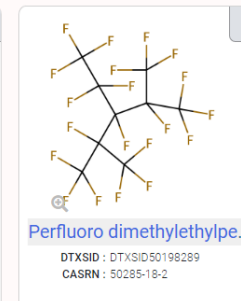
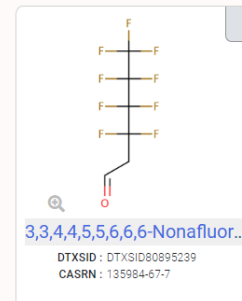
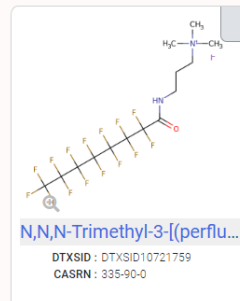
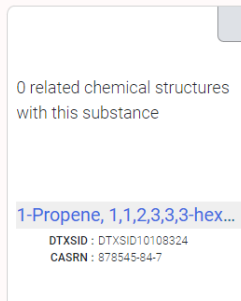
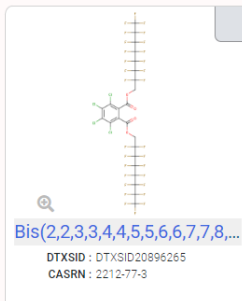
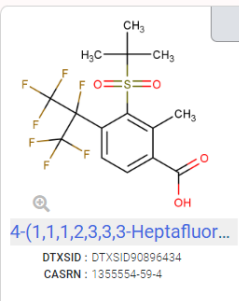
TITLE INFO

FILTER

EXPORT

PREFERRED VIEW

Showing 4729 of 4729 chemicals



What is the definition of PFAS now?

- According to OECD “PFAS are fluorinated substances that contain at least one fully fluorinated methyl or methylene carbon atom (without any H/Cl/Br/I atom attached to it)”
- This means, that “with a few noted exceptions, any chemical with at least a perfluorinated methyl group ($-\text{CF}_3$) or a perfluorinated methylene group ($-\text{CF}_2-$) is a PFAS.”

- Under the overly broad & simple definitions there are MILLIONs of PFAS in PubChem

Select classification

Search selected classification by

PubChem: PFAS and Fluorinated Compounds in PubChem

Keyword

Enter desired search term

Search

Classification description (from PubChem)

A classification tree to browse per- and polyfluoroalkyl substances (PFAS) and other fluorinated compounds in PubChem. The 'OECD PFAS definition' node contains PubChem content matching the OECD PFAS definition of saturated CF₂ (Report ENV/CBC/MONO(2021)25 from 9 July 2021). The 'Organofluorine compounds' node contains organofluorine compounds in PubChem as defined in the same report. The 'Other diverse fluorinated compounds' node helps explore a wide variety of other fluorinated compounds. The 'PFAS and fluorinated compound collections' node gathers several collections of PFAS and/or fluorinated compounds from various resources.

Update: 06/16/22 11:56:01 [More...](#)

Data type counts to display

Display zero count nodes?

Filter by Entrez History

None

Compound

Yes

No

Choose one

Browse PubChem: PFAS and Fluorinated Compounds in PubChem Tree

PFAS and Fluorinated Compounds in PubChem

OECD PFAS definition

Organofluorine compounds

Other diverse fluorinated compounds

PFAS and fluorinated compound collections

19,405,024

6,094,574

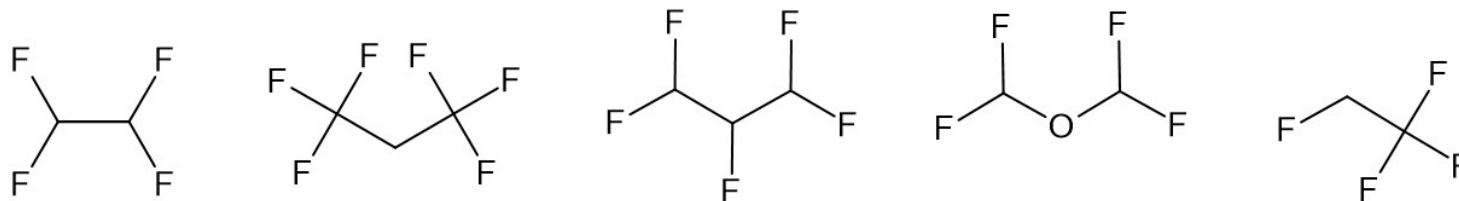
19,254,827

107,376

1,785,539

- Definitions of PFAS can differ across research groups and scientific publications
- Simple definitions are too all-encompassing but are used to capture small fluorinated chemicals of concern
- No consistent PFAS definition across the scientific community, but areas of heightened concern, e.g.,
 - PFOA, PFOS & chemicals that break down to these PFAS
 - Chemicals or polymers containing C7-C11 linear perfluoro chains
 - Organics with high degree of fluorination relative to carbon
- We employ a structure-based approach for defining membership in PFAS lists
 - Substances containing specific substructural elements

PFAS Structure List v4 (10,776)



List Details

Description: List consists of all DTXSID records with a structure assigned, and using a set of substructural filters based on community input. The substructural filters ([visible here](#)) are designed to be simple, reproducible and transparent, yet general enough to encompass the largest set of structures having sufficient levels of fluorination to potentially impart PFAS-type properties. Relative to the previous list ([PFSSTRUCTv3](#)) the trifluoroacetate substructure has been removed from the substructure filters.

Number of Chemicals: 10776

Search Results

SEND 7000 TO BATCH SEARCH

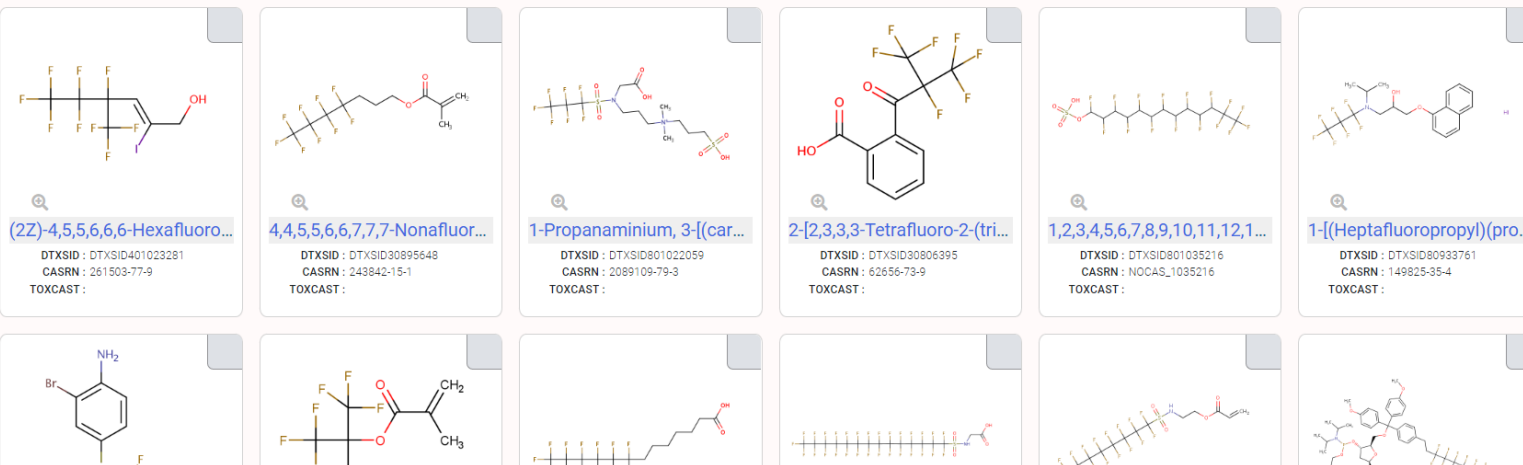
TILE INFO

FILTER

EXPORT

PREFERRED VIEW

Showing 7000 of 7000 chemicals



But we continue to iterate

Navigation Panel to PFAS Structure Lists

Search for chemical by systematic name, synonym, CAS number, DTXSID or chemical structure

☐ Identifier substring search

List Details

Description: PFAS Structure lists are versioned iteratively and this description may be updated (e.g., August 2021). For the versioned lists please use the hyperlinked lists below.

[PFASSTRUCTV4 - August 2021](#) This list

[PFASSTRUCTV3 - August 2020](#)

[PFASSTRUCTV2 - November 2019](#)

[PFASSTRUCTV1 - March 2018](#)

Number of Chemicals: 10776

Building a “PFAS List”

- Definitions of PFAS can differ across research groups and scientific publications
- Simple definitions are too all-encompassing but are used to capture small fluorinated chemicals of concern
- No consistent PFAS definition across the scientific community, but areas of heightened concern, e.g.,
 - PFOA, PFOS & chemicals that break down to these PFAS
 - Chemicals or polymers containing C7-C11 linear perfluoro chains
 - Organics with high degree of fluorination relative to carbon
- We employ a structure-based approach for defining membership in PFAS lists
 - Substances containing specific substructural elements
 - Substances with specific “substrings” to represent PFAS elements in UVCB chemicals

Chemical Substances of Unknown or Variable Composition, Complex Reaction Products and Biological Materials (UVCB Substance) on the TSCA Inventory

This paper is a compendium of information related to the broad class of chemical substances referred to as UVCBs for the Toxic Substances Control Act (TSCA) Chemical Substance Inventory. These chemical substances cannot be represented by unique structures and molecular formulas.

- There are thousands of polymers with PFAS monomeric units
- The process of mapping monomers to polymers requires careful curation efforts
- There are a number of biodegradable PFAS (e.g., food-contact materials)

PFAS "UVCB Chemicals"

1258 in PFASDEV1 list

List Details

Description: List of PFAS chemicals without explicit structures - polymers and other UVCB chemicals. The list was assembled by searching on the following substring list: Perfluoro, Polyfluoro, Fluoroethylene, Fluoropropylene, Fluorobutene, Fluoropolymer, "Ethene, 1,1,2,2-tetrafluoro" (the PTFE monomer unit), Chlorotrifluoroethylene, Difluoromethylene, Vinyl fluoride, Tetrafluoro, Pentafluoro, Hexafluoro, Heptafluoro, Octafluoro, Nonafluoro and Decafluoro and filtering out distinct chemical structures. This will retain Markush structure representations. This list remains under constant curation and expansion. Last Updated (August 8th 2021)

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey

☐ Identifier substring search

List Details

Description: List of PFAS chemicals without explicit structures - polymers and other UVCB chemicals. The list was assembled by searching on the following substring list: Perfluoro, Polyfluoro, Fluoroethylene, Fluoropropylene, Fluorobutene, Fluoropolymer, "Ethene, 1,1,2,2-tetrafluoro" (the PTFE monomer unit), Chlorotrifluoroethylene, Difluoromethylene, Vinyl fluoride, Tetrafluoro, Pentafluoro, Hexafluoro, Heptafluoro, Octafluoro, Nonafluoro and Decafluoro and filtering out distinct chemical structures. This will retain Markush structure representations. This list remains under constant curation and expansion. Last Updated (August 8th 2021)

Number of Chemicals: 1258

Search Results

SEND 1258 TO BATCH SEARCH

TILE INFO

FILTER

EXPORT

PREFERRED VIEW

Showing 1258 of 1258 chemicals

0 related chemical structures
with this substance

[212013-59-7 \(name too lo...](#)

DTXSID : DTXSID08082609
CASRN : 212013-59-7
TOXCAST :



[Alkyl iodides C4-20, gam...](#)

DTXSID : DTXSID060881973
CASRN : 68188-12-5
TOXCAST :

0 related chemical structures
with this substance

[2-Propenoic acid, 2-methy...](#)

DTXSID : DTXSID020897651
CASRN : 1221681-75-9
TOXCAST :

0 related chemical structures
with this substance

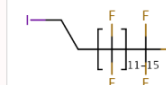
[Ethene, tetrafluoro-, oxidiz...](#)

DTXSID : DTXSID40108079
CASRN : 274918-03-5
TOXCAST :

0 related chemical structures
with this substance

[Hexene, undecafluoro\(4-s...](#)

DTXSID : DTXSID080893452
CASRN : 134344-15-3
TOXCAST :



[Alkyl iodides, C14-18, ga...](#)

DTXSID : DTXSID40881996
CASRN : 68390-32-9
TOXCAST :

Example PFAS-UVCBs

0 related chemical structures with this substance Ethene, tetrafluoro-, oxidiz... DTXSID : DTXSID40108079 CASRN : 274918-03-5 TOXCAST :	0 related chemical structures with this substance Ethanol, 2-amino-, reactio... DTXSID : DTXSID50897689 CASRN : 161212-14-2 TOXCAST :	0 related chemical structures with this substance Ethene, 1,1,2,2-tetrafluoro... DTXSID : DTXSID001023560 CASRN : 1638852-33-1 TOXCAST :	0 related chemical structures with this substance Borate(1-), tetrahydro-, so... DTXSID : DTXSID701023547 CASRN : 1214752-86-9 TOXCAST :	0 related chemical structures with this substance Ethene, tetrafluoro-, oxidiz... DTXSID : DTXSID00108075 CASRN : 274917-96-3 TOXCAST :
0 related chemical structures with this substance Methanol, reaction produc... DTXSID : DTXSID00897674 CASRN : 161308-20-9 TOXCAST :	0 related chemical structures with this substance Ethene, 1,1,2,2-tetrafluoro... DTXSID : DTXSID501023565 CASRN : 1664368-38-0 TOXCAST :	0 related chemical structures with this substance Hexanoic acid, 6-amino-, r... DTXSID : DTXSID00897699 CASRN : 161212-12-0 TOXCAST :	0 related chemical structures with this substance Methanol, reaction produc... DTXSID : DTXSID80897692 CASRN : 161308-25-4 TOXCAST :	0 related chemical structures with this substance 2-Propenoic acid, 2-methy... DTXSID : DTXSID80897632 CASRN : 161308-18-5 TOXCAST :

↳ Ethene, tetrafluoro-, oxidized, polymd., reduced, decarboxylated, C6 fraction
274917-96-3 | DTXSID00108075

↳ 1-Propene, 1,1,2,3,3,3-hexafluoro-, polymer with 1,1-difluoroethene, ethene, 1,1,2,2-tetrafluoroethene and 1,1,2-trifluoro-2-(trifluoromethoxy)ethene
149935-01-3 | DTXSID00108732



1-Hexene, 3,3,4,4,5,5,6,6,6-nonafluoro-, polymer with ethene and 1,1,2,2-tetrafluoroethene

1-Hexene, 3,3,4,4,5,5,6,6,6-nonafluoro-, polymer with ethene and 1,1,2,2-tetrafluoroethene

68258-85-5 | DTXSID50880596

Searched by DTXSID50880596.

Related Substances

 Search Results


SEND 4 TO BATCH SEARCH

TILE INFO


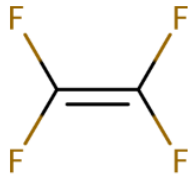

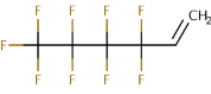

FILTER

EXPORT

PREFERRED VIEW

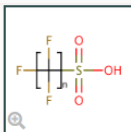


Showing 4 of 4 chemicals

<div>Searched Chemical</div> <p>3 related chemical structures with this substance</p> <p>1-Hexene, 3,3,4,4,5,5,6,6,6-...</p> <p>DTXSID : DTXSID50880596 CASRN : 68258-85-5 TOXCAST :</p>	<div>Monomer</div> <p>$\text{H}_2\text{C}=\text{CH}_2$</p> <p></p> <p>Ethylene</p> <p>DTXSID : DTXSID1026378 CASRN : 74-85-1 TOXCAST :</p>	<div>Monomer</div> <p></p> <p></p> <p>Tetrafluoroethylene</p> <p>DTXSID : DTXSID6021325 CASRN : 116-14-3 TOXCAST :</p>	<div>Monomer</div> <p></p> <p></p> <p>3,3,4,4,5,5,6,6,6-Nonafluor...</p> <p>DTXSID : DTXSID6047575 CASRN : 19430-93-4 TOXCAST :</p>
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“Markush” Chemical Categories

- PFOS is a linear perfluoroalkyl sulfonate

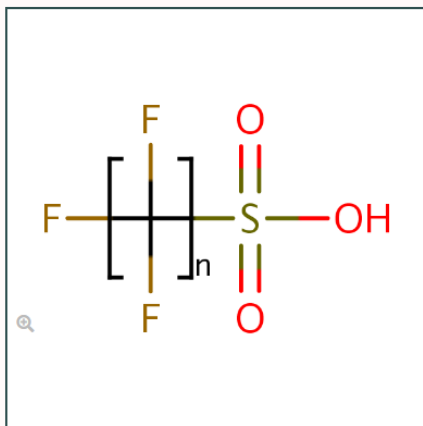


Perfluoroalkyl (linear) sulfonic acids

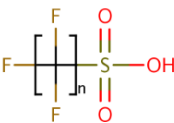
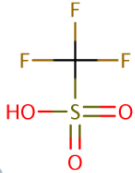


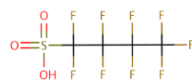





NOCAS_892979 | DTXSID70892979

Searched by DTXSID70892979.

Chemical Details



Showing 21 of 21 chemicals

<p>Searched Chemical</p>  <p>Perfluoroalkyl (linear) sulf...</p> <p>DTXSID : DTXSID70892979 CASRN : NOCAS_892979 TOXCAST :</p>	<p>Markush Child</p>  <p>Trifluoromethanesulfonic ...</p> <p>DTXSID : DTXSID2044397 CASRN : 1493-13-6 TOXCAST : 1/235</p>	<p>Markush Child</p>  <p>Perfluoroethanesulfonic a...</p> <p>DTXSID : DTXSID30870511 CASRN : 354-88-1 TOXCAST :</p>	<p>Markush Child</p>  <p>Perfluoropropanesulfonic ...</p> <p>DTXSID : DTXSID30870531 CASRN : 423-41-6 TOXCAST :</p>	<p>Markush Child</p>  <p>Perfluorobutanesulfonic a...</p> <p>DTXSID : DTXSID5030030 CASRN : 375-73-5 TOXCAST :</p>
<p>Markush Child</p>  <p>Perfluoropentanesulfonic ...</p> <p>DTXSID : DTXSID8062600 CASRN : 2706-91-4 TOXCAST :</p>	<p>Markush Child</p>  <p>Perfluorohexanesulfonic a...</p> <p>DTXSID : DTXSID7040150 CASRN : 355-46-4 TOXCAST :</p>	<p>Markush Child</p>  <p>Perfluoroheptanesulfonic ...</p> <p>DTXSID : DTXSID8059920 CASRN : 375-92-8 TOXCAST :</p>	<p>Markush Child</p>  <p>Perfluorooctanesulfonic a...</p> <p>DTXSID : DTXSID3031864 CASRN : 1763-23-1 TOXCAST : 298/1272</p>	<p>Markush Child</p>  <p>Perfluorononanesulfonic ...</p> <p>DTXSID : DTXSID8071356 CASRN : 68259-12-1 TOXCAST :</p>
<p>Markush Child</p>	<p>Markush Child</p>	<p>Markush Child</p>	<p>Markush Child</p>	<p>Markush Child</p>

PFAS Categories - evolves as new classes are added

List Details

Description: List of registered DSSTox "category substances" representing Per- and Polyfluoroalkyl Substances (PFAS) categories created using ChemAxon's Markush structure-based query representations. Markush categories can be broad and inclusive of more specific categories or can represent a unique category not overlapping with other registered categories. Each PFAS category registered with a unique DTXSID is considered a generalized substance or "parent ID" that can be associated with one or many "child IDs" (i.e. many parent-child mappings) within the full DSSTox database. These category DTXSIDs can be used to search and retrieve all currently registered DSSTox substances within the category group, and offer an objective, transparent and reproducible structure-based means of defining a category of chemicals. This list and the corresponding category mappings are undergoing continuous curation and expansion.

Number of Chemicals: 112

Search Results

SEND 112 TO BATCH SEARCH

TILE INFO

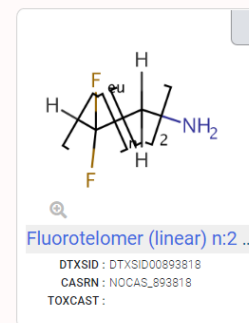
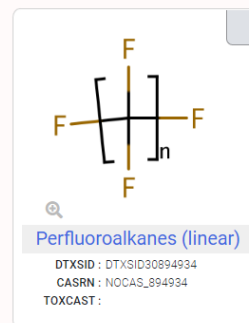
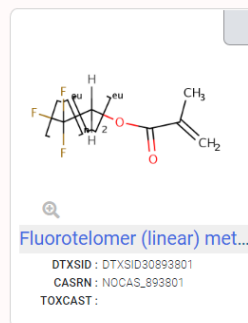
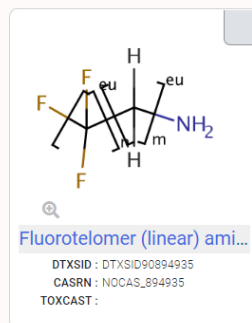
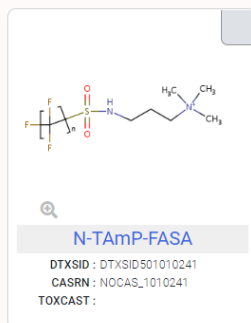
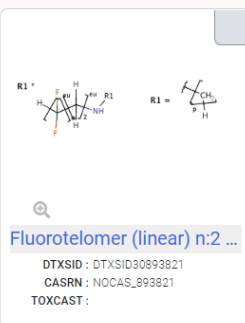
FILTER

EXPORT

PREFERRED VIEW

Grid icon


Showing 112 of 112 chemicals



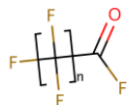
PFAS Categories in Development (112 categories so far... and evolving)

Vol. 127, No. 1 | Brief Communication

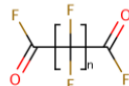
A Chemical Category-Based Prioritization Approach for Selecting 75 Per- and Polyfluoroalkyl Substances (PFAS) for Tiered Toxicity and Toxicokinetic Testing

Grace Patlewicz , Ann M. Richard, Antony J. Williams, Christopher M. Grulke, Reeder Sams, Jason Lambert, Pamela D. Noyes, Michael J. DeVito, Ronald N. Hines, Mark Strynar, Annette Guiseppi-Elie, and Russell S. Thomas

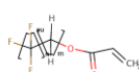
Published: 11 January 2019 | **CID:** 014501 | <https://doi.org/10.1289/EHP4555> | **Cited by:** 17



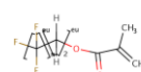
Perfluoroalkyl acyl fluorides
CASRN:NOCAS_893647
DTXSID:DTXSID10893647



Perfluoroalkyl symmetric diacyl fluorides
CASRN:NOCAS_893648
DTXSID:DTXSID70893648



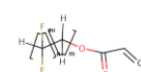
Fluorotelomer (linear) acrylates
CASRN:NOCAS_893800
DTXSID:DTXSID70893800



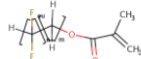
Fluorotelomer (linear) methacrylates
CASRN:NOCAS_893801
DTXSID:DTXSID30893801



Fluorotelomer (linear) n2 alcohols
CASRN:NOCAS_893802
DTXSID:DTXSID90893802



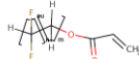
Fluorotelomer (linear) n2 acrylates (-CH...
CASRN:NOCAS_893803
DTXSID:DTXSID50893803



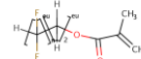
Fluorotelomer (linear) methacrylates (-C...
CASRN:NOCAS_893804
DTXSID:DTXSID10893804



Fluorotelomer (linear) alcohols (-CHF2)
CASRN:NOCAS_893805
DTXSID:DTXSID70893805



Fluorotelomer (linear) acrylates (-CHF2)
CASRN:NOCAS_893814
DTXSID:DTXSID60893814



Fluorotelomer (linear) n2 methacrylates ...
CASRN:NOCAS_893815
DTXSID:DTXSID20893815



Fluorotelomer (linear) n2 alcohols (-CHF2)
CASRN:NOCAS_893816
DTXSID:DTXSID80893816



Fluorotelomer (linear) n2 amines (prima...
CASRN:NOCAS_893817
DTXSID:DTXSID40893817

BATCH SEARCHING

- Search ***thousands*** of chemicals based on CASRN, names and identifiers
- Harvest *en masse* the data available for single chemicals – properties, tox data, chemical relationships, category mappings, presence in lists

Batch Searches

Batch Search

1 Select Input Type(s)

- ☒ Substance Identifiers
- ☒ Chemical Name
 - ☒ CASRN
 - ☐ InChIKey
 - ☐ DSSTox Substance ID
- ☐ DSSTox Compound ID
- ☐ InChIKey Skeleton
- ☐ MS-Ready Formula(e)
- ☐ Exact Formula(e)
- ☐ Monoisotopic Mass

2 Enter Identifiers to Search

(Please enter one identifier per line and limit the number of identifiers to 10,000 or less)

15347-57-6
124-04-9
7778-50-9
Butan-2-yl (2,4,5-trichlorophenoxy)acetate
Antimony potassium tartrate trihydrate
77-47-4
107-92-6
3813-14-7

3

 DISPLAY ALL CHEMICALS

or

 CHOOSE EXPORT OPTIONS

Customize Export Results

4

 CHOOSE EXPORT FORMAT ▾

Your file will be exported in Microsoft Excel Format (.xlsx)

☐ Select All columns available




Chemical Identifiers

- ☒ DTXSID
- ☒ Chemical Name
- ☐ DTXCID
- ☐ CAS-RN
- ☐ InChIKey
- ☐ IUPAC Name

Metadata

- ☐ Curation Level Details
- ☐ Safety Data
- ☐ NHANES/Predicted Exposure
- ☐ Data Sources
- ☐ Include ToxVal Data Availability
- ☐ Assay Hit Count
- ☐ Number of PubMed Articles

Presence in Lists

<input type="checkbox"/>	Title	Description
<input type="checkbox"/>		
<input type="checkbox"/>	40CFR1164 	40 CFR 116.4 Designation of Hazardous Substances (Above Ground Storage Tanks)
<input type="checkbox"/>	40CFR355 	40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities
<input type="checkbox"/>	ACSREAG 	LIST: ACS Reagent Chemicals

Four Chemical Trends Will Shape the Next Decade's Directions in Perfluoroalkyl and Polyfluoroalkyl Substances Research

Matthias Kotthoff* and Mark Bücking

Department Environmental and Food Analysis, Fraunhofer Institute for Molecular Biology and Applied Ecology,
Schmallenberg, Germany

- 1. **Mobility**: A wide and dynamic distribution of short chain PFAS due to their high polarity, persistency and volatility. → **QSAR Predictions**
- 2. **Substitution of regulated substances**: The ban or restrictions of individual molecules will lead to a replacement with substitutes of similar concern. → **Database content and Markush Enumeration**
- 3. **Increase in structural diversity of existing PFAS molecules**: Introduction of e.g., hydrogens and chlorine atoms instead of fluorine, as well as branching and cross-linking lead to a high versatility of unknown target molecules. → **Database content**
- 4. **Unknown “Dark Matter”**: The amount, identity, formation pathways, and transformation dynamics of polymers and PFAS precursors are largely unknown. → **Working with agency analytical scientists and collaborators to link and host data**

- CompTox Chemicals Dashboard supports PFAS research at EPA in numerous ways
 - Delivery of curated lists of PFAS chemicals (growing)
 - Flexible search capabilities – support for Mass Spec
 - Relationships in the data enrich navigation between chemicals
- Ongoing research efforts for PFAS chemicals
 - Continue harvesting physicochemical & fate and transport data
 - Classification approaches and Markush representations
 - Expand available toxicity data and integration to systematic review data as it becomes available

ORIGINAL RESEARCH article

Front. Environ. Sci., 05 April 2022
Sec. Toxicology, Pollution and the
Environment

<https://doi.org/10.3389/fenvs.2022.850019>

This article is part of the Research Topic

Environmental Pollution and Toxicity of Emerging Per- and
Polyfluoroalkyl Substances (PFASs)

[View all Articles >](#)

Assembly and Curation of Lists of Per- and Polyfluoroalkyl Substances (PFAS) to Support Environmental Science Research



Antony J. Williams^{1*},



Linda G. T. Gaines²,



Christopher M. Grulke^{1†},



Charles N. Lowe¹,



Gabriel F. B. Sinclair³,



Vicente Samano⁴,



Inthirany

Thillainadarajah⁴,



Bryan Meyer⁴,



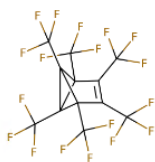
Grace Patlewicz¹ and



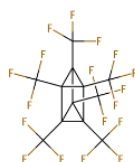
Ann M. Richard¹

The story isn't over...

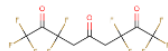
- Latest dashboard release >1.2M substances
- New PFASSTRUCTv5 list, *adjusting* definition to address missed chemicals: **~15k**



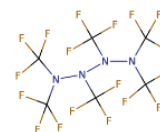
Tricyclo(3.1.0.0~2.6~)hex-3-ene, 1,2,3,4,5,6-hexafluoro-
DTXSID:DTXSID30176722
CASRN:22186-64-7
TOXCAST:-



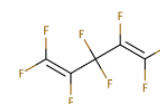
Perfluorohexamethylprismane
DTXSID:DTXSID30177274
CASRN:22736-20-5
TOXCAST:-



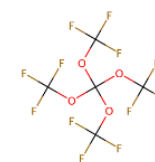
1,1,1,3,3,7,7,9,9-Decafluorononane-2,5-dione
DTXSID:DTXSID60435490
CASRN:28393-78-4
TOXCAST:-



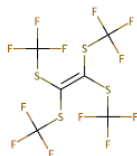
Hexakis(trifluoromethyl)tetraazane
DTXSID:DTXSID20471975
CASRN:313-40-6
TOXCAST:-



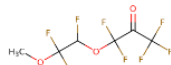
1,1,2,3,3,4,5,5-Octafluoropenta-1,4-diene
DTXSID:DTXSID30529779
CASRN:3109-87-3
TOXCAST:-



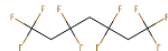
Tetrakis(trifluoromethoxy)methane
DTXSID:DTXSID40552018
CASRN:92639-87-7
TOXCAST:-



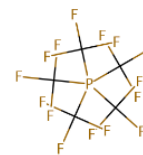
Tetrakis(trifluoromethyl)sulfanylene
DTXSID:DTXSID50577656
CASRN:13003-40-2
TOXCAST:-



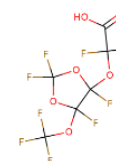
1,1,1,3,3-Pentafluoro-3-(1,2,2-trifluoro-2-methoxyethyl)propane
DTXSID:DTXSID40748237
CASRN:88457-04-9
TOXCAST:-



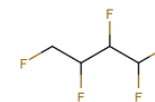
1,1,1,3,3,5,5,7,7-Decafluoroheptane
DTXSID:DTXSID20776331
CASRN:162102-06-9
TOXCAST:-



Pentakis(trifluoromethyl)-lambda⁵-phosphorane
DTXSID:DTXSID20837133
CASRN:827027-07-6
TOXCAST:-

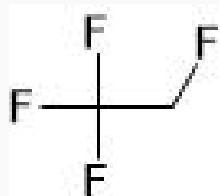


Perfluoro(2-[5-methoxy-1,3-dioxolan-4-yl]ethyl)propanoic acid
DTXSID:DTXSID60882627
CASRN:1190931-41-9
TOXCAST:-

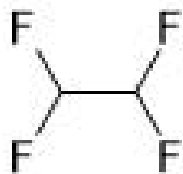


1,1,2,3,4-Pentafluorobutane
DTXSID:DTXSID50931113
CASRN:141529-32-0
TOXCAST:-

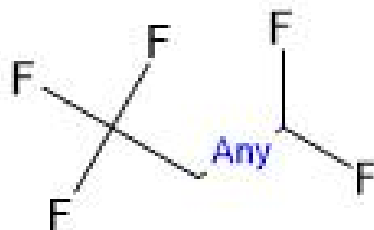
- 30% F based on fraction of molecular formula excluding H
 - For example, for $C_6HF_9O_6$, the F percent excluding H contained in the formula would be $9F/(6C + 9F + 6O) = 42\%$
 - OECD (2021) argued against using a weight percent F, but this is simply a count percent and excludes atomic weight
- Or contains one of four substructures
 - For substructure 4, Q can be B, O, N, P, S, or Si



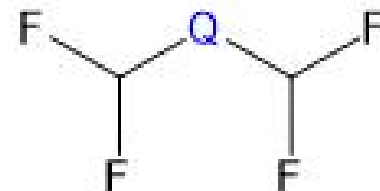
(1)



(2)



(3)

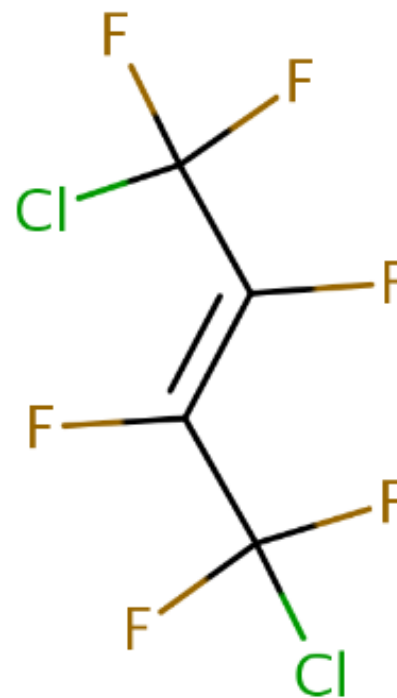
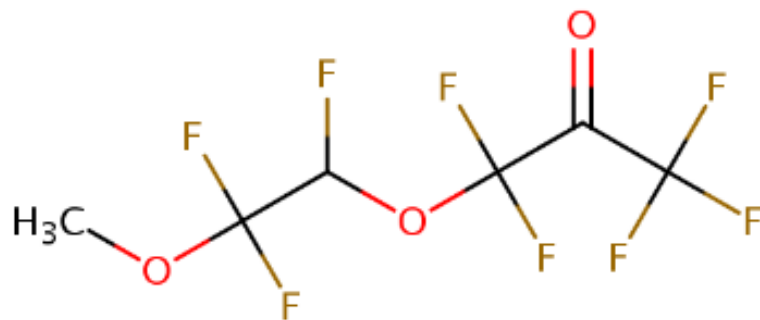


(4)

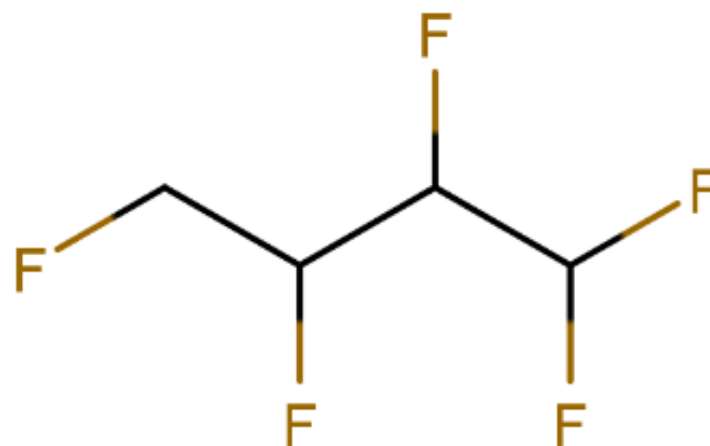
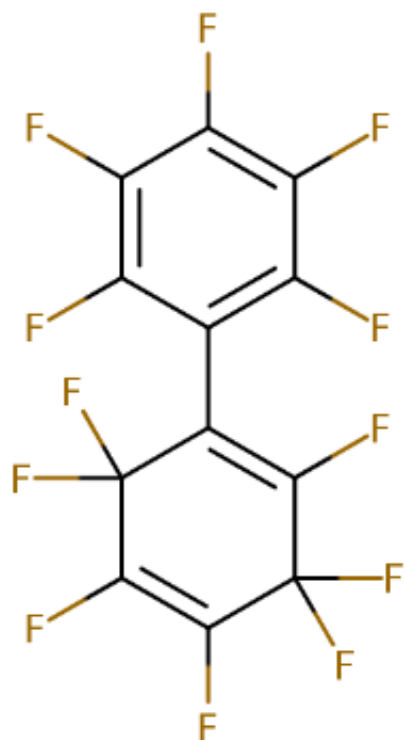
I know a PFAS when I see one

Justice Potter Stewart, in concurring on the decision in *Jacobellis v. Ohio*, 378 U.S. 184, stated **“I shall not today attempt further to define the kinds of material I understand to be embraced within that shorthand description; and perhaps I could never succeed in intelligibly doing so. But I know it when I see it, and the motion picture involved in this case is not that.”**

Structures Included in Proposed New Definition



Structures Included in Proposed New Definition



PFAS CCL5...another tweak

WATER|EPA: Chemical Contaminants - CCL 5 PFAS subset

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey

☐ Identifier substring search

List Details

Description: The Contaminant Candidate List (CCL) is a list of contaminants that are currently not subject to any proposed or promulgated national primary drinking water regulations, but are known or anticipated to occur in public water systems. Contaminants listed on the CCL may require future regulation under the Safe Drinking Water Act (SDWA). EPA announced the Final Contaminant Candidate List 5 on November 2nd 2022. For the purpose of CCL 5, excluding PFOA and PFOS, the structural definition of per- and polyfluoroalkyl substances (PFAS) includes chemicals that contain at least one of these three structures: 1) R-(CF₂)-CF(R')R'', where both the CF₂ and CF moieties are saturated carbons, and none of the R groups can be hydrogen 2) R-CF₂OCF₂-R', where both the CF₂ moieties are saturated carbons, and none of the R groups can be hydrogen 3) CF₃C(CF₃)RR', where all the carbons are saturated, and none of the R groups can be hydrogen The Final CCL 5 includes 69 chemicals or chemical groups and 12 microbial contaminants. The CCL 5 list is available [here](#)

Number of Chemicals: 10239

- Don't worry about the details – definitions can be adjusted

- The research discussed in this presentation is part of EPA's overall efforts to rapidly expand the scientific foundation for understanding and managing risk from PFAS.
- For more information on EPA's efforts to address PFAS, please visit the following websites
 - EPA PFAS Action Plan - <https://www.epa.gov/pfas/epas-pfas-action-plan>
 - EPA PFAS Research - <https://www.epa.gov/chemical-research/research-and-polyfluoroalkyl-substances-pfas>

Acknowledgements

- CCTE colleagues – Ann Richard, Grace Patlewicz, Charlie Lowe, Nate Charest
- CCTE Curation Team
- Linda Gaines, EPA-OLEM

Antony Williams

NCCT, US EPA Office of Research and Development,

Williams.Antony@epa.gov

ORCID: <https://orcid.org/0000-0002-2668-4821>

Williams et al. *J Cheminform* (2017) 9:61
DOI 10.1186/s13321-017-0247-6


 Journal of Cheminformatics

DATABASE

Open Access

The CompTox Chemistry Dashboard: a community data resource for environmental chemistry



Antony J. Williams^{1*} , Christopher M. Grulke¹, Jeff Edwards¹, Andrew D. McEachran², Kamel Mansouri^{1,2,4}, Nancy C. Baker³, Grace Patlewicz¹, Imran Shah¹, John F. Wambaugh¹, Richard S. Judson¹ and Ann M. Richard¹

<https://doi.org/10.1186/s13321-017-0247-6>