

US-EPA Comptox Chemicals Dashboard: information hub for PFAS chemicals

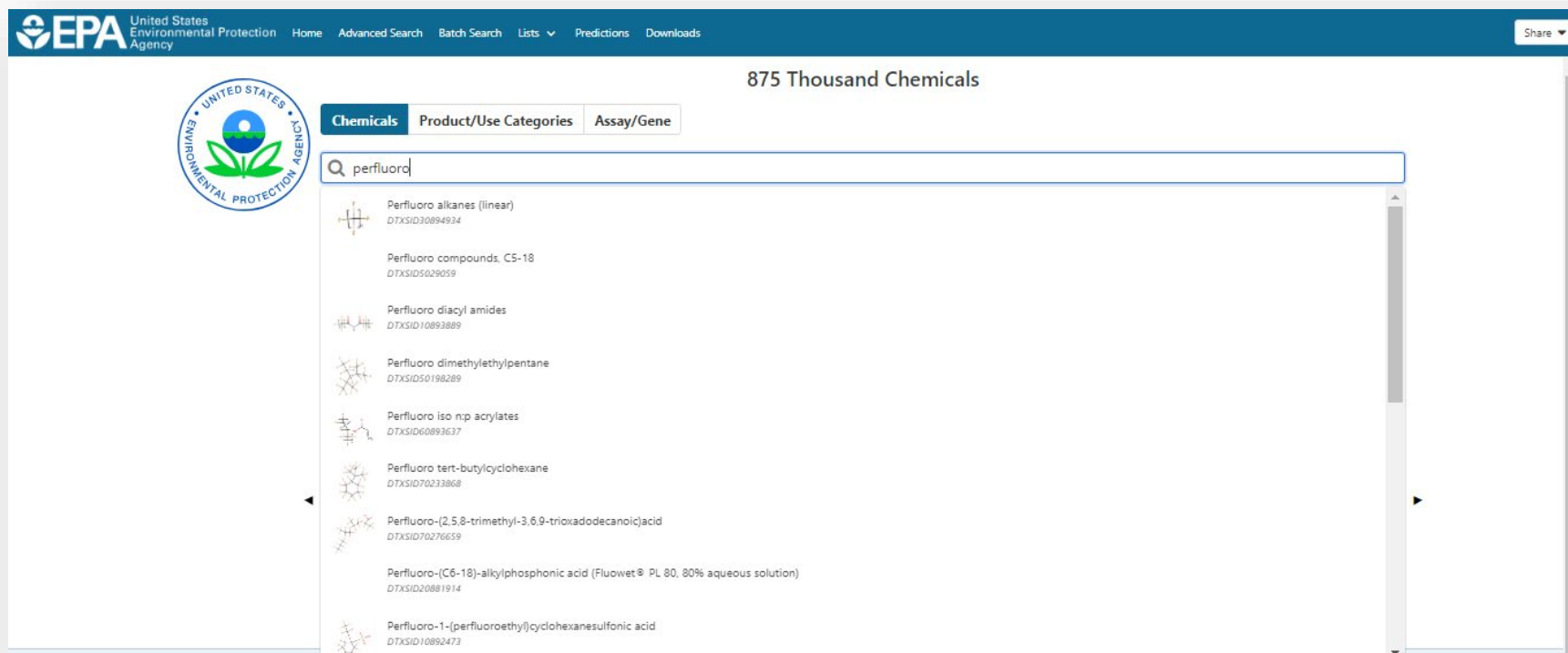
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The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA


CompTox Chemicals Dashboard

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



The screenshot displays the CompTox Chemicals Dashboard interface. At the top, the EPA logo and navigation links (Home, Advanced Search, Batch Search, Lists, Predictions, Downloads) are visible. The main header shows "875 Thousand Chemicals". Below this, there are tabs for "Chemicals", "Product/Use Categories", and "Assay/Gene". A search bar contains the text "perfluor". The search results are listed below, each with a chemical structure icon, a name, and a DTXSID:

- Perfluoro alkanes (linear)
DTXSID30894934
- Perfluoro compounds, C5-18
DTXSID5029059
- Perfluoro diacyl amides
DTXSID10893889
- Perfluoro dimethylethylpentane
DTXSID50198289
- Perfluoro iso n-p acrylates
DTXSID60893637
- Perfluoro tert-butylcyclohexane
DTXSID70233868
- Perfluoro-(2,5,8-trimethyl-3,6,9-trioxadodecanoic)acid
DTXSID70276659
- Perfluoro-(C6-18)-alkylphosphonic acid (Fluowet® PL 80, 80% aqueous solution)
DTXSID20881914
- Perfluoro-1-(perfluoroethyl)cyclohexanesulfonic acid
DTXSID10892473


United States
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[Lists](#)
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Search all data


PFASListed in OECD Global Database

Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by DSSTox Substance Id.

DETAILS
EXECUTIVE SUMMARY
PROPERTIES
ENV. FATE/TRANSPORT
HAZARD
ADME
EXPOSURE
BIOACTIVITY
SIMILAR COMPOUNDS
GENRA (BETA)
RELATED SUBSTANCES
SYNONYMS
LITERATURE
LINKS
COMMENTS



Wikipedia

Perfluorooctanesulfonic acid (conjugate base perfluorooctanesulfonate) (PFOS) is an anthropogenic fluorosurfactant and global pollutant. PFOS was the key ingredient in Scotchgard, a fabric protector made by 3M, and numerous stain repellents. It was added to Annex B of the Stockholm Convention on Persistent Organic Pollutants in May 2009. PFOS can be synthesized in industrial production or result from the degradation of precursors. PFOS levels that have been detected in wildlife

Read more

Intrinsic Properties

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Quality Control Notes

UNITED STATES
Discover
Connect
Ask

Are there Similar Compounds?

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search all data

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

TOXCAST: SUMMARY

EDSP21

TOXCAST/TOX21


PUBCHEM

TOXCAST: MODELS

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES




Perfluorooctanesulfonic acid
1763-23-1 | DTXSID3031864
Searched by Synonym from Valid Source.

Searched with a similarity threshold of 0.8

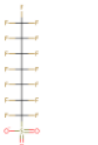
83 chemicals

Select all Download Send to Batch Search Similarity ⌵ ⌵ DTXSID CASRN TOXCAST Similarity ⌵

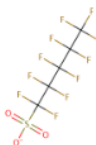
Hide chemicals that are: Filter by Name or CASRN




Heptadecafluorooctane-1-(2H)sulfonic a...
DTXSID: DTXSID00892720
CASRN: NOCAS_892720
TOXCAST: -
Similarity: 1.00



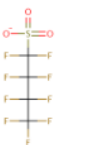
Perfluoroheptanesulfonate
DTXSID: DTXSID20892505
CASRN: 146689-46-5
TOXCAST: -
Similarity: 1.00




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




Magnesium bis(heptadecafluorooctanes...
DTXSID: DTXSID80881314
CASRN: 91036-71-4
TOXCAST: -
Similarity: 1.00



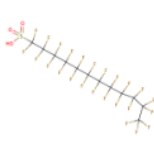
Perfluorobutanesulfonate
DTXSID: DTXSID60873015
CASRN: 45187-15-3
TOXCAST: -
Similarity: 1.00



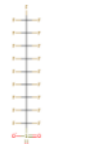
Perfluorododecylsulfonate



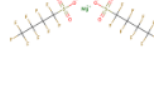
Perfluorobutanesulfonate



Perfluorododecylsulfonic acid



Perfluoropentanesulfonate



Magnesium nonafluorobutanesulfonate

3

Relationships in the data

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search all data

Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by Synonym from Valid Source.


13 chemicals

Select all Download Send to Batch Search Relationship DTXSID PubChem CPDAT

Hide chemicals that are: Filter by Name or CASR

Relationship	Chemical Name	DTXSID	PubChem	CPDAT
Searched Chemical	Perfluorooctanesulfonic acid	DTXSID: DTXSID3031864	PubChem: 68	CPDAT: 10
Markush Parent	Perfluoroalkyl sulfonates	DTXSID: DTXSID70892979	PubChem: 0	CPDAT: 0
Markush Parent	Perfluoroalkyl (linear) sulfonates	DTXSID: DTXSID30896832	PubChem: 0	CPDAT: 0
Predecessor: Component	3 related chemical structures with this substance	Mixture of PFOS and PFOA DTXSID: DTXSID20872963	PubChem: 0	CPDAT: 0
Predecessor: Component	3 related chemical structures with this substance	1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5... DTXSID: DTXSID40880545	PubChem: 0	CPDAT: 0
Component	Perfluorooctanesulfonate	DTXSID: DTXSID80108992	PubChem: 10	
Salt Form	Lithium perfluorooctanesulfonate	DTXSID: DTXSID2032421	PubChem: 32	
Salt Form	Potassium perfluorooctanesulfonate	DTXSID: DTXSID8037706	PubChem: 59	
Salt Form	Ammonium perfluorooctanesulfonate	DTXSID: DTXSID9067435	PubChem: 17	
Salt Form	Tetraethylammonium perfluorooctanesulfonate	DTXSID: DTXSID5069128	PubChem: 42	

Batch Searches

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Agency**

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

Batch Search?

Step 1 Step 2 Step 3 Step 4 Step 5 Step 6

Step Six: Click "Download"

Please enter one identifier per line

Select Input Type(s)

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

Display All Chemicals Download Chemical Data

Select Output Format:

Excel

Download

Customize Results

- ☐ Select All
- ☐ Select All in Lists

Enter Identifiers to Search (searches should be limited to <5000 identifiers)


107-02-8
79-06-1
107-13-1
309-00-2
107-18-6
62-53-3
7631-89-2
1327-53-3
7784-46-5
26628-22-8

Presence in Lists:

- ☐ 40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities
- ☐ AEGLs: Acute Exposure Guideline Levels

A List of Lists of Chemicals

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


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Home Advanced Search Batch Search Lists ▼ Predictions Downloads

Share ▼ Search all data

Select List

Download ▼ Columns ▼

 Copy Filtered Lists URL

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
EPAPFAS75S1	PFAS EPA: List of 75 Test Samples (Set 1)	2018-06-29	74	PFAS list corresponds to 75 samples (Set 1) submitted for initial testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program.
EPAPFAS75S2	PFAS EPA: List of 75 Test Samples (Set 2)	2019-02-21	75	PFAS list corresponds to a second set of 75 samples (Set 2) submitted for testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program.
EPAPFASCAT	PFAS EPA Structure-based Categories	2018-06-29	64	List of registered DSSTox "category substances" representing PFAS categories created using ChemAxon's Markush structure-based query representations.
EPAPFASINSOL	PFAS EPA: Chemical Inventory Insoluble in DMSO	2018-06-29	43	PFAS chemicals included in EPA's expanded ToxCast chemical inventory found to be insoluble in DMSO above 5mM.
EPAPFASINV	PFAS EPA: ToxCast Chemical Inventory	2018-06-29	430	PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing.
EPAPFASRL	PFAS EPA: Cross-Agency Research List	2017-11-16	199	EPAPFASRL is a manually curated listing of mainly straight-chain and branched PFAS (Per- & Poly-fluorinated alkyl substances) compiled from various internal, literature and public sources by EPA researchers and program office representatives.
PFASKEMI	PFAS: List from the Swedish Chemicals Agency (KEMI) Report	2017-02-09	2416	Perfluorinated substances from a Swedish Chemicals Agency (KEMI) Report on the occurrence and use of highly fluorinated substances.
PFASMASTER	PFAS Master List of PFAS	2018-07-26	5061	PFASMASTER is a consolidated list of PFAS substances spanning and bounded by the below lists of current

The OECD List of PFAS

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

PFAS: Listed in OECD Global Database

☐ Identifier substring search

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

4729 chemicals

Select all

Download

Send to Batch Search

Default

DTXSID

PubChem

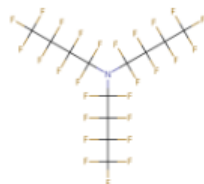
CPDAT

Hide chemicals that are:

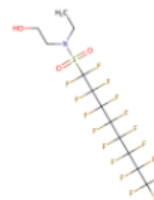
Filter by Name or CASRN



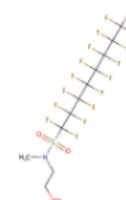
Perfluorooctanesulfonyl fluoride
DTXSID: DTXSID5027140
PubChem: 71
CPDAT: 6



Perfluorotributylamine
DTXSID: DTXSID0027141
PubChem: 71
CPDAT: 0

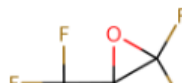


N-Ethyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide
DTXSID: DTXSID6027426
PubChem: 54
CPDAT: 3



N-Methyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide
DTXSID: DTXSID7027831
PubChem: 24
CPDAT: 16

0 related chemical
structures with this



PFAS "Structure List"

PFAS|EPA: PFAS structures in DSSTox (update August 2020)

☐ Identifier substring search

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.

Number of Chemicals: 8163

8163 chemicals

Select all



Send to Batch Search

Default



DTXSID

CASRN

TOXCAST

Hide chemicals that are:

Filter by Name or CASRN



Enflurane

DTXSID:DTXSID1020562

CASRN:13838-16-9

TOXCAST:0/235



1,1,1,2-Tetrafluoroethane

DTXSID:DTXSID1021324

CASRN:811-97-2

TOXCAST:-



Tetrafluoroethylene

DTXSID:DTXSID6021325

CASRN:116-14-3

TOXCAST:-

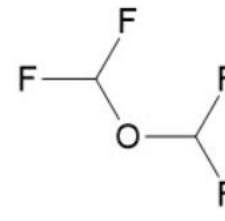
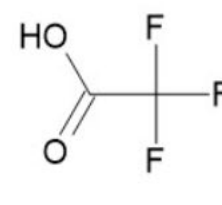
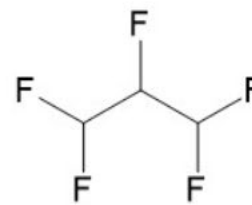
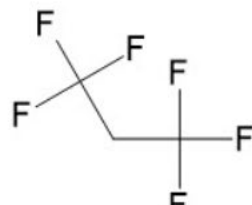
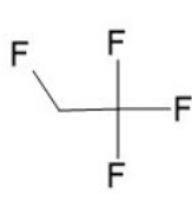
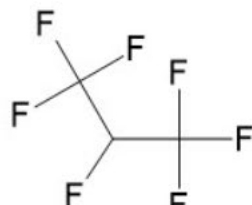
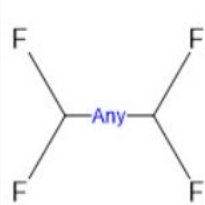


2H-Perfluoro-2-propanol

DTXSID:DTXSID1022134

CASRN:920-66-1

TOXCAST:-



PFAS without structures

PFAS|EPA PFAS chemicals without explicit structures

☐ 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, Decafluoro, Dodecafluoro and filtering out chemical structures. This list remains under constant curation and expansion. Last Updated (September 16th 2020)

Number of Chemicals: 1089

1089 chemicals

Select all

 Download

Send to Batch Search

Default



DTXSID

CASRN

TOXCAST

Hide chemicals that are:

Filter by Name or CASRN



0 related chemical
structures with this
substance

[Perfluoro compounds, C5-18](#)
DTXSID:DTXSID5029059
CASRN:86508-42-1
TOXCAST:7/235

1 related chemical
structure with this
substance

[Poly\(difluoromethylene\), alpha-chloro-o...](#)
DTXSID:DTXSID2042301
CASRN:79070-11-4
TOXCAST:-

1 related chemical
structure with this
substance

[Poly\(difluoromethylene\), alpha-fluoro-o...](#)
DTXSID:DTXSID7042302
CASRN:65530-66-7
TOXCAST:-

1 related chemical
structure with this
substance

[Polytetrafluoroethylene](#)
DTXSID:DTXSID7047724
CASRN:9002-84-0
TOXCAST:-

Example PFAS-UVCBs

0 related chemical
structures with this
substance

Ethene, tetrafluoro-, oxidized, polymd., ...
DTXSID: DTXSID00108075
CASRN: 274917-96-3

0 related chemical
structures with this
substance

Sulfonamides, C4-8-alkane, perfluoro, ...
DTXSID: DTXSID00108095
CASRN: 160901-25-7

0 related chemical
structures with this
substance

1-Propene, 1,1,2,3,3,3-hexafluoro-, pol...
DTXSID: DTXSID00108732
CASRN: 149935-01-3

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

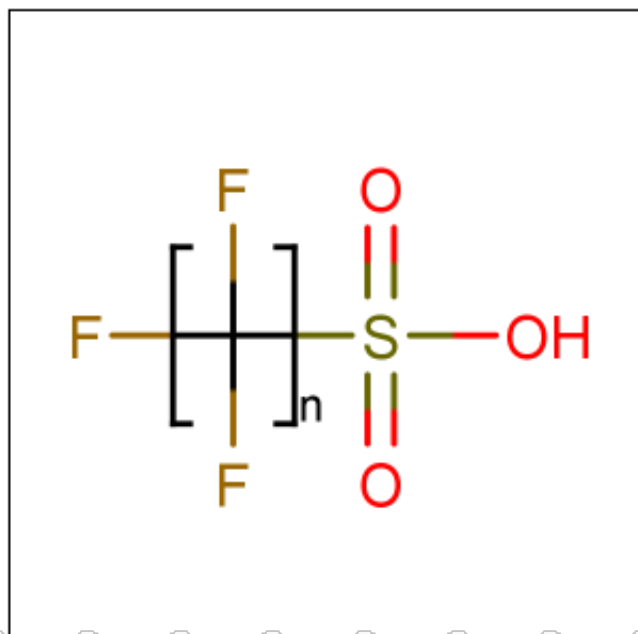
↳ 1-Propene, 1,1,2,3,3,3-hexafluoro-, polymer with 1,1-difluoroethene, ethene, 1,1,2,2-tetrafluoroethene and 1,1,2-trifluoro-2-(trifluoromethoxy)ethene
149935-01-3 | DTXSID00108732

- PFOS is a member of linear perfluoroalkyl sulfonates

Perfluoroalkyl sulfonates

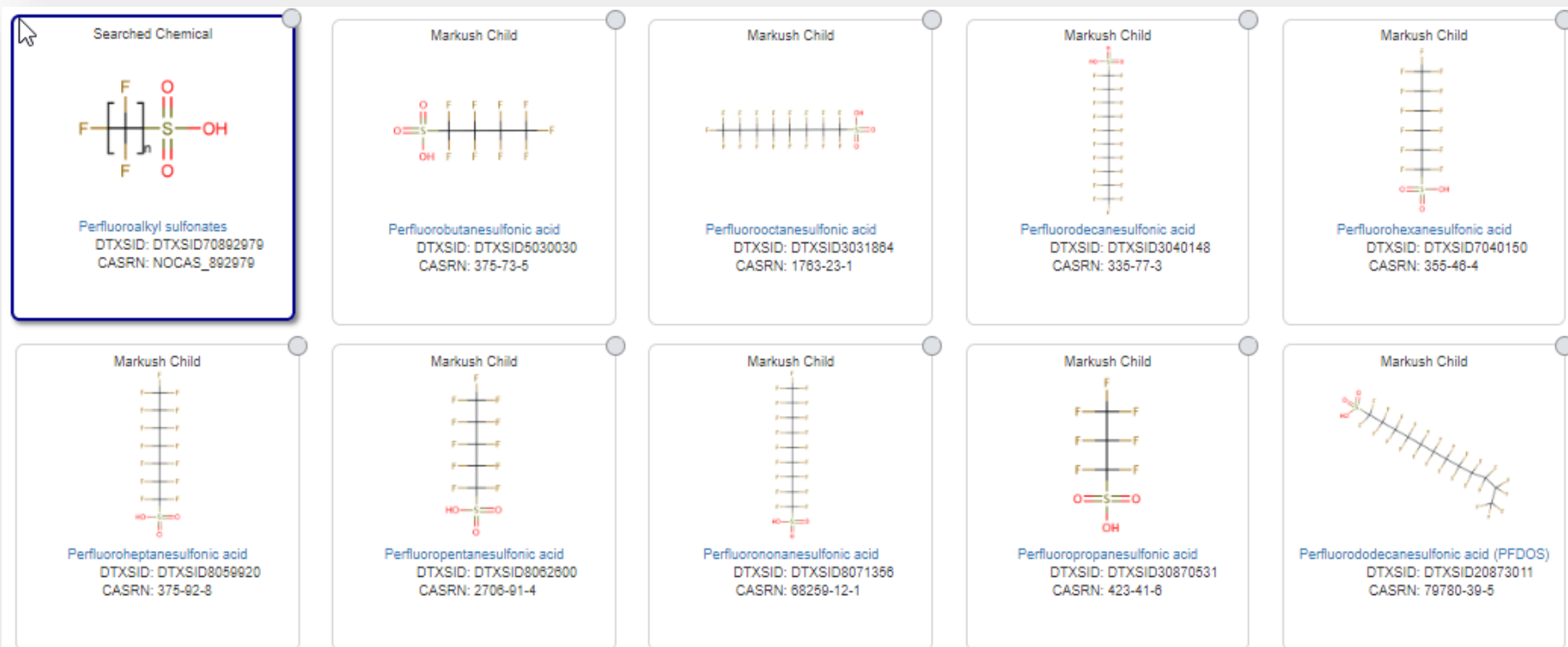
NOCAS_892979 | DTXSID70892979

Searched by DSSTox Substance Id.



...and their Markush Children...

- Linear perfluoroalkyl sulfonates has children...



PFAS Categories in Development

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 is undergoing continuous curation and expansion.

Number of Chemicals: 64

64 chemicals

Select all

Download

Send to Batch Search

Default



DTXSID

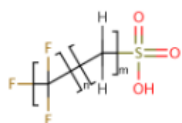
PubChem

CPDAT



Hide chemicals that are:

Filter by Name or CASRN



Fluorotelomer (linear) sulfonic acids

DTXSID: DTXSID50892558

PubChem: 0

CPDAT: 0

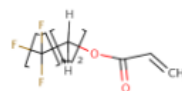


Fluorotelomer (linear) alcohols

DTXSID: DTXSID10893581

PubChem: 0

CPDAT: 0

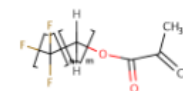


Fluorotelomer (linear) n:2 acrylates

DTXSID: DTXSID70893582

PubChem: 0

CPDAT: 0



Fluorotelomer (linear) n:2 methacrylates

DTXSID: DTXSID30893583

PubChem: 0

CPDAT: 0

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 Journal of Cheminformatics

DATABASE

Open Access

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



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