

PFAS Chemistry: Range, Complexity, Groupings, and the CompTox Chemicals Dashboard

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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

September 2020

The Science of PFAS, Virtual Conference

- **A publicly accessible website** delivering access:
 - ~882,000 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 consumer products containing chemicals
 - Links to other agency websites and public data resources
 - “Literature” searches for chemicals using public resources
 - “Batch searching” for thousands of chemicals
- **Over 10,000 of the chemicals are classed as PFAS Chemicals**







CompTox Chemicals Dashboard

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



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

The screenshot displays the EPA CompTox Chemicals Dashboard interface. At the top, the EPA logo and navigation links (Home, Advanced Search, Batch Search, Lists, Predictions, Downloads) are visible. The dashboard title "CompTox Chemicals Dashboard" and the count "882 Thousand Chemicals" are prominently displayed. A search bar contains the text "perfluorid". Below the search bar, a list of search results is shown, each with a chemical structure icon, a name, and a DTXSID number.

Chemicals	Product/Use Categories	Assay/Gene
	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 potassium salt DTXSID301023652	
	Perfluoro-(2,5,8-trimethyl-3,6,9-trioxadodecanoic)acid DTXSID70276659	

Substring search “perfluoro”

- Substring search ~2000 chemicals

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

Search Results

Searched with 'Synonym Substring': Perfluoro

2098 chemicals

Select all Download Send to Batch Search DTXSID CASRN TOXCAST

Hide chemicals that are: Filter by Name or CASRN

<p>N-(Carboxymethyl)-N,N-dimethyl-3-(1H-perfluorooctyl)propanamide DTXSID:DTXSID001009316 CASRN:NOCAS_1009316 TOXCAST:-</p>	<p>Sodium 8-chloroperfluoro-1-octanesulfonate DTXSID:DTXSID001009916 CASRN:NOCAS_1009916 TOXCAST:-</p>	<p>Perfluoroalkyl (linear) alkyl ethers DTXSID:DTXSID001015365 CASRN:NOCAS_1015365 TOXCAST:-</p>	<p>Perfluorooctanesulfonamide lithium salt DTXSID:DTXSID001016256 CASRN:76752-79-9 TOXCAST:-</p>	0 related chemical structures with this substance	<p>Perfluoro(3-[[1-(ethenyloxy)propan-2-yl]oxy]propyl)dimethylphosphine oxide DTXSID:DTXSID001023627 CASRN:870707-45-2 TOXCAST:-</p>
<p>Perfluoro-3,7,11-trioxatetradecane DTXSID:DTXSID001023689 CASRN:122076-00-0 TOXCAST:-</p>	<p>Perfluoro-2-methyl-2-(pentyloxy)pentane DTXSID:DTXSID001023784 CASRN:93200-92-1 TOXCAST:-</p>	0 related chemical structures with this substance	<p>1H,1H,2H,2H-Perfluorooctyldimethylchlorosilane DTXSID:DTXSID00145182 CASRN:102488-47-1 TOXCAST:-</p>	<p>(2-(F-Hexyl)ethyl) dimorpholinophosphine oxide DTXSID:DTXSID00158474 CASRN:134051-89-1 TOXCAST:-</p>	<p>Monopotassium monoperfluorooxyl DTXSID:DTXSID00164454 CASRN:150033-28-6 TOXCAST:-</p>

Substring search “perfluoro” “Explicit” structures

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Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

Search Results

Searched with 'Synonym Substring': Perfluoro

2098 chemicals

Select all Download Send to Batch Search DTXSID DTXSID CASRN TOXCAST

Hide chemicals that are: Filter by Name or CASRN

N-(Carboxymethyl)-N,N-dimethyl-3-(1H,1H,2H,2H-perfluorooctyl)sulfonamide lithium salt

DTXSID:DTXSID001009316
CASRN:NOCAS_1009316
TOXCAST:-

Perfluorooctanesulfonamide lithium salt

DTXSID:DTXSID001016256
CASRN:76752-79-9
TOXCAST:-

0 related chemical structures with this substance

Ethene, 1-[difluoro(trifluoromethoxy)methyl]-

DTXSID:DTXSID001023572
CASRN:870707-45-2
TOXCAST:-

Perfluoro(3-[[1-(ethenoxy)propan-2-yl]oxy]propyl)sulfonate

DTXSID:DTXSID001023627
CASRN:77545-07-4
TOXCAST:-

1H,1H,2H,2H-Perfluorooctyldimethylchlorosilane

DTXSID:DTXSID00145182
CASRN:102488-47-1
TOXCAST:-

(2-(F-Hexyl)ethyl) dimorpholinophosphine oxide

DTXSID:DTXSID00158474
CASRN:134051-89-1
TOXCAST:-

Monopotassium monoperfluorohexyl sulfonate

DTXSID:DTXSID00164454
CASRN:150033-28-6
TOXCAST:-

emical
ith this
ce

perfluoro, N,...
D00108095
11-25-7

Substring search “perfluoro” “Markush” representations

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Search all data

Search Results

Searched with 'Synonym Substring': Perfluoro

2098 chemicals

Select all Download Send to Batch Search DTXSID CASRN TOXCAST

Hide chemicals that are: Filter by Name or CASRN

N-(Carboxymethyl)-N,N-dimethyl-3-(1H-imidazol-2-yl)propan-2-yl...
DTXSID:DTXSID001009316
CASRN:NOCAS_1009316
TOXCAST:-

Sodium 8-chloroperfluoro-1-octanesulfonate
DTXSID:DTXSID001009916
CASRN:NOCAS_1009916
TOXCAST:-

Perfluoro-3,7,11-trioxatetradecane
DTXSID:DTXSID001023689
CASRN:122076-00-0
TOXCAST:-

Perfluoro-2-methyl-2-(pentyloxy)pentane
DTXSID:DTXSID001023784
CASRN:93200-92-1
TOXCAST:-

Perfluoroalkyl (linear) alkyl ethers
DTXSID:DTXSID001015365
CASRN:NOCAS_1015365
TOXCAST:-

Perfluoro(3-[[1-(ethenoxy)propan-2-yl]oxy]methyl)propan-2-yl...
DTXSID:DTXSID001023627
CASRN:77545-07-4
TOXCAST:-

Monopotassium monoperfluorohexyl ether
DTXSID:DTXSID00164454
CASRN:150033-28-6
TOXCAST:-

Substring search “perfluoro” “UVCB” chemicals

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

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

Search Results

Searched with 'Synonym Substring': Perfluoro

2098 chemicals

Select all Download Send to Batch Search DTXSID CASRN TOXCAST

Hide chemicals that are: Filter by Name or CASRN

<p>N-(Carboxymethyl)-N,N-dimethyl-3-(1H,1H,2H,2H-perfluorooctyl)acrylamide DTXSID:DTXSID001009316 CASRN:NOCAS_1009316 TOXCAST:-</p>	<p>Sodium 8-chloroperfluoro-1-octanesulfonate DTXSID:DTXSID001009916 CASRN:NOCAS_1009916 TOXCAST:-</p>	<p>Perfluoroalkyl (linear) alkyl ethers DTXSID:DTXSID001015365 CASRN:NOCAS_1015365 TOXCAST:-</p>	<p>Perfluorooctanesulfonamide lithium salt DTXSID:DTXSID001016752 CASRN:76752-79-9 TOXCAST:-</p>
<p>Perfluoro-3,7,11-trioxatetradecane DTXSID:DTXSID001023689 CASRN:122076-00-0 TOXCAST:-</p>	<p>Perfluoro-2-methyl-2-(pentyloxy)pentane DTXSID:DTXSID001023784 CASRN:93200-92-1 TOXCAST:-</p>	<p>0 related chemical structures with this substance</p>	<p>1H,1H,2H,2H-Perfluorooctyldimethylsilane DTXSID:DTXSID001024888 CASRN:102488-47-2 TOXCAST:-</p>

0 related chemical structures with this substance

Ethene, 1-[difluoro(trifluoromethoxy)me...

DTXSID:DTXSID001023572

CASRN:870707-45-2

TOXCAST:-

United States
Environmental Protection
Agency

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PFASOECD
PFAS Listed in OECD Global
Database

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

Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864
Searched by DSSTox Substance Id.

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

Physicochemical properties

Property



Summary



Summary

LogP: Octanol-Water

Melting Point

Boiling Point

Water Solubility

Vapor Pressure

Flash Point

Surface Tension

Index of Refraction

Molar Refractivity

Polarizability

Density

Molar Volume

Thermal Conductivity

Viscosity

Henry's Law

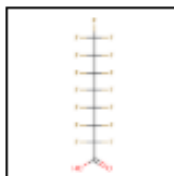
LogKoa: Octanol-Air

Summary

Search query

Average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
		3.43	3.32	2.40 to 3.64	
	156	138	153 to 156	125 to 157	°C
		360	200	343 to 401	°C
		1.00e-3	5.26e-4	5.44e-4 to 1.31e-3	mol/L
		3.43e-7	-	6.83e-8 to 2.59e-6	mmHg
		190	-	188 to 192	°C
			-	46.0	dyn/cm
			-	1.60	
			-	68.2	cm^3
			-	27.0	Å^3
		1.17	-	1.14 to 1.20	g/cm^3
			-	200	cm^3
			-	150	mW/(m^2K)

Experimental Data




Perfluorooctanoic acid


335-67-1 | DTXSID8031865

Searched by Synonym from Valid Source.

Property


 Water Solubility ▼

Water Solubility

 Download Summary ▼

Type	Average	Median	Range
Experimental	1.56e-2	1.56e-2	8.21e-3 to 2.29e-2
Predicted	1.01e-2	6.38e-5	6.27e-8 to 4.01e-2

Experimental

 Download Experimental Data ▼

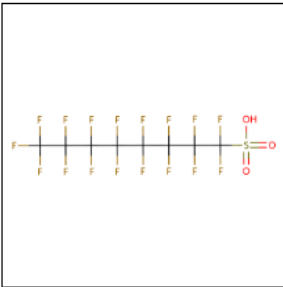
Source	Result	Experimental Details
3M_PFOA_Sheet	8.21e-3	
ATSDR_Perfluoroalkyl_Cheminfo	2.29e-2	
Danish_EPA_PFOA_Report_2005	2.29e-2	
Danish_EPA_SCPFAS_Report_2015	8.21e-3	

Detailed QSAR Prediction Reports

OPERA Models: Vapor Pressure

Perfluorooctanesulfonic acid
1763-23-1 | DTXSID3031864

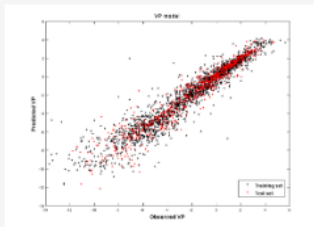
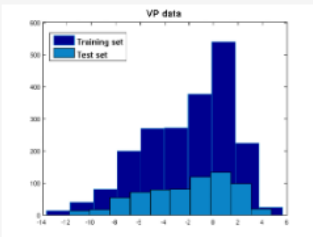
Print PDF



Model Results

Predicted values: 1.49e-2 mmHg
Global applicability domain: **Outside**
Local applicability domain index: 0.338
Confidence level: 0.286

Model Performance

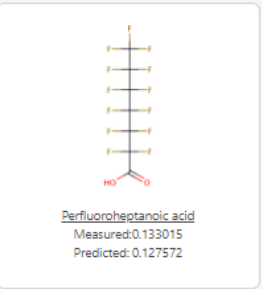
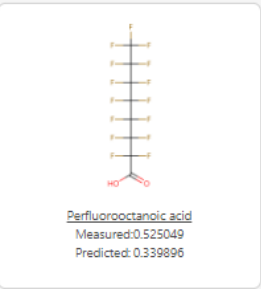
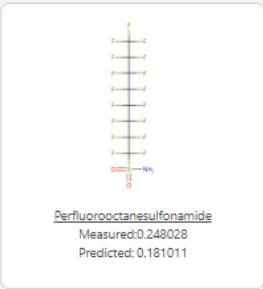
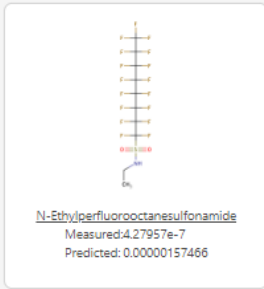


QMRF

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.910	1.08	0.910	1.08	0.920	1.00

Nearest Neighbors from the Training Set



Environmental Toxicology and Chemistry—Volume 39, Number 4—pp. 775–786, 2020

Received: 8 October 2019 | Revised: 30 October 2019 | Accepted: 3 February 2020

775

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

Hazard Data – Human and Eco

 **United States
Environmental Protection
Agency**

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DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

► EXPOSURE

► BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES


SYNONYMS


► LITERATURE

LINKS

COMMENTS

DataType









 Ecotox Effect Level ▼

 Download ▼

Human

Eco

Columns ▼

More ▼	Priority ▼	Toxval type ▼	Subtype ▼	Risk assessment class ▼	Value ▼	Units ▼	Study type ▼	Exposure route ▼	Species ▼	Subsource ▼	Source ▼
	6	EC10	-	growth:acute	2.6	mg/L	growth	static	sea urchin, echinoderm	J. Environ. Monit.14(5): 1375-1382	ECOTOX
	6	EC10	-	mortality:acute	3.2	mg/L	mortality	static	mysid	J. Environ. Monit.14(5): 1375-1382	ECOTOX
	6	EC50	-	mortality:acute	141.7	mg/L	mortality	renewal	black sandshell	Environ. Toxicol. Chem.31(7): 1611-1620	ECOTOX
	6	EC50	-	mortality:acute	158.1	mg/L	mortality	renewal	lamp-mussel	Environ. Toxicol. Chem.31(7): 1611-1620	ECOTOX
	6	EC50	-	mortality:acute	6.9	mg/L	mortality	static	mysid	J. Environ. Monit.14(5): 1375-1382	ECOTOX
	6	EC50	-	mortality:acute	158.1	mg/L	mortality	renewal	lamp-mussel	Environ. Toxicol. Chem.31(7): 1611-1620	ECOTOX
	6	EC50	-	growth:acute	20	mg/L	growth	static	sea urchin, echinoderm	J. Environ. Monit.14(5): 1375-1382	ECOTOX
	6	EC50	-	mortality:acute	158.1	mg/L	mortality	renewal	black sandshell	Environ. Toxicol. Chem.31(7): 1611-1620	ECOTOX

What is PFOS Called?

Synonyms, CASRNs and more

DETAILS

EXECUTIVE SUMMARY

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► EXPOSURE

► BIOACTIVITY

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GENRA (BETA)

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Perfluorooctanesulfonic acid

Heptadecafluorooctane-1-sulfonic acid

1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-

1763-23-1 **Active CASRN**

Heptadecafluorooctanesulfonic acid

1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-

1-Octanesulfonic acid, heptadecafluoro-

EF 101

heptadecafluorooctane-1-sulfonic acid

heptadecafluorooctane-1-sulphonic acid

PFOS

EINECS 217-179-8

1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-Heptadecafluoro-1-octanesulfonic acid

Share

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Search query

Quality
Valid
Valid
Valid
Valid
Valid
Valid
Valid
Valid
Valid
Good
Other
Other
Other
Other
Other
Other
Other

- 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?

128 chemicals >0.8 match factor

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

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ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

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COMMENTS

128 chemicals

Select all Download Send to Batch Search Similarity CASRN DTXSID Molecular Formula Hide chemicals that are: Filter by Name or CASRN

Perfluorobutanesulfonate
CASRN:45187-15-3
DTXSID:DTXSID60873015
Molecular Formula:C4F9O3S

Perfluorobutanesulfonic acid
CASRN:375-73-5
DTXSID:DTXSID5030030
Molecular Formula:C4HF9O3S

Perfluoropentanesulfonate
CASRN:175905-36-9
DTXSID:DTXSID70892479
Molecular Formula:C5F11O3S

Perfluoropentanesulfonic acid
CASRN:2706-91-4
DTXSID:DTXSID8062600
Molecular Formula:C5HF11O3S

Perfluorohexanesulfonate
CASRN:108427-53-8
DTXSID:DTXSID80873012
Molecular Formula:C6F13O3S

Perfluorohexanesulfonic acid
CASRN:355-46-4
DTXSID:DTXSID7040150
Molecular Formula:C6HF13O3S

Perfluoroheptanesulfonate
CASRN:146689-46-5
DTXSID:DTXSID20892505
Molecular Formula:C7F15O3S

Perfluoroheptanesulfonic acid
CASRN:375-92-8
DTXSID:DTXSID8059920
Molecular Formula:C7HF15O3S


Perfluorooctanesulfonate
CASRN:45298-90-6
DTXSID:DTXSID80108992
Molecular Formula:C8F17O3S

Heptadecafluorooctane-1-(2H)sulfonic a...
CASRN:NOCAS_892720
DTXSID:DTXSID00892720
Molecular Formula:C8DF17O3S

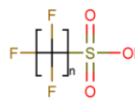
Relationships in the data

DETAILS
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ADME
EXPOSURE
BIOACTIVITY
SIMILAR COMPOUNDS
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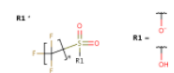
13 chemicals
Select all Download Send to Batch Search Relationship
DTXSID CASRN TOXCAST
Hide chemicals that are: Filter by Name or CASRN

Searched Chemical


Perfluorooctanesulfonic acid
DTXSID:DTXSID3031864
CASRN:1763-23-1
TOXCAST:267/1129

Markush Parent


Perfluoroalkyl sulfonates
DTXSID:DTXSID70892979
CASRN:NOCAS_892979
TOXCAST:-

Markush Parent


Perfluoroalkyl (linear) sulfonates
DTXSID:DTXSID30896832
CASRN:NOCAS_896832
TOXCAST:-

Predecessor: Component


3 related chemical structures with this substance

Mixture of PFOS and PFOA
DTXSID:DTXSID20872963
CASRN:NOCAS_872963
TOXCAST:-


Predecessor: Component

3 related chemical structures with this substance


1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,...
DTXSID:DTXSID40880545
CASRN:64202-77-3
TOXCAST:-

Component



Perfluorooctanesulfonate
DTXSID:DTXSID80108992
CASRN:45298-90-6
TOXCAST:-

Salt Form


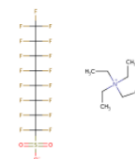
Lithium perfluorooctanesulfonate
DTXSID:DTXSID2032421
CASRN:29457-72-5
TOXCAST:33/238

Salt Form


Potassium perfluorooctanesulfonate
DTXSID:DTXSID8037706
CASRN:2795-39-3
TOXCAST:179/820

Salt Form


Ammonium perfluorooctanesulfonate
DTXSID:DTXSID9067435
CASRN:29081-56-9
TOXCAST:-

Salt Form


Tetraethylammonium perfluorooctanesulfonate
DTXSID:DTXSID5069128
CASRN:56773-42-3
TOXCAST:-

16

9 salt forms of PFOS (and the ion)

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Mixtures, Components, and Neutralized Forms of Perfluorooctanesulfonic acid

9 chemicals

Select all Download Send to Batch Search Default DTXSID PubChem CPDAT

Hide chemicals that are: Filter by Name or CASR

Chemical Name	DTXSID	PubChem	CPDAT
Perfluorooctanesulfonic acid	DTXSID03031864	68	10
Lithium perfluorooctanesulfonate	DTXSID2032421	32	14
Potassium perfluorooctanesulfonate	DTXSID8037706	59	18
Ammonium perfluorooctanesulfonate	DTXSID9067435	17	5
Bis(2-hydroxyethyl)ammonium perfluoro...	DTXSID2072049	19	4
Perfluorooctanesulfonate	DTXSID80108992	10	5
Sodium perfluorooctanesulfonate	DTXSID50635462	13	0
Heptadecafluorooctane-1-(² H)sulfonic a...	DTXSID00892720	0	0
heptadecafluoro(1,2,3,4-13C4)octane-1-...	DTXSID80894101	0	0

CHEMICAL LISTS OF PFAS

A List of Lists of Chemicals

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

Download

Columns

10

PFAS

Copy Filtered Lists URL

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
PFASSTRUCT	PFAS EPA: PFAS structures in DSSTox (update August 2020)	2020-09-04	8163	List of all structures contained in DSSTox bounded by multiple substructure filters used to identify PFAS (per- and polyfluorinated substances)
PFASMASTER	PFAS Master List of PFAS Substances	2018-06-29	5070	PFASMASTER is a consolidated list of PFAS substances spanning and bounded by the below lists of current interest to researchers and regulators worldwide.
PFASOECD	PFAS: Listed in OECD Global Database	2018-05-16	4729	OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances, (PFASs) listing more than 4700 new PFAS
PFASOECDNA	NORMAN: List of PFAS from the OECD Curated by Nikiforos Alygizakis	2019-05-03	3213	List of PFAS released by the OECD, provided by Zhanyun Wang, curated and mapped to structures by Nikiforos Alygizakis
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.
PFASDEV1	PFAS EPA PFAS chemicals without explicit structures	2020-08-29	1097	List of PFAS chemicals without explicit structures - polymers and other UVCB chemicals
PFASTRIER	PFAS Community-Compiled List (Trier et al., 2015)	2017-07-16	597	PFASTRIER community-compiled public listing of PFAS (Trier et al, 2015)
EPAPFASINV	PFAS EPA: ToxCast Chemical Inventory	2018-06-29	430	PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing.
PFASNORDIC	PFAS: Nordic PFAS Report 2019	2020-01-31	386	List of PFAS cited in the Nordic Working Paper on Per- and polyfluoroalkylether substances:identity, production and use (2020)
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.

- 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/>

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/>

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

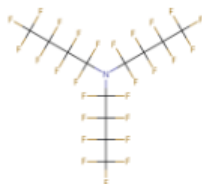
CPDAT

Hide chemicals that are:

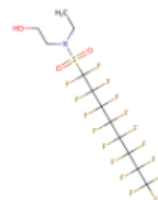
Filter by Name or CASRN



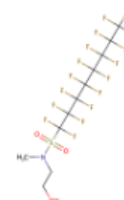
Perfluorooctanesulfonyl fluoride
DTXSID: DTXSID5027140
PubChem: 71
CPDAT: 6



Perfluorotributylamine
DTXSID: DTXSID0027141
PubChem: 71
CPDAT: 0

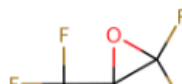


N-Ethyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide
DTXSID: DTXSID6027426
PubChem: 54
CPDAT: 3



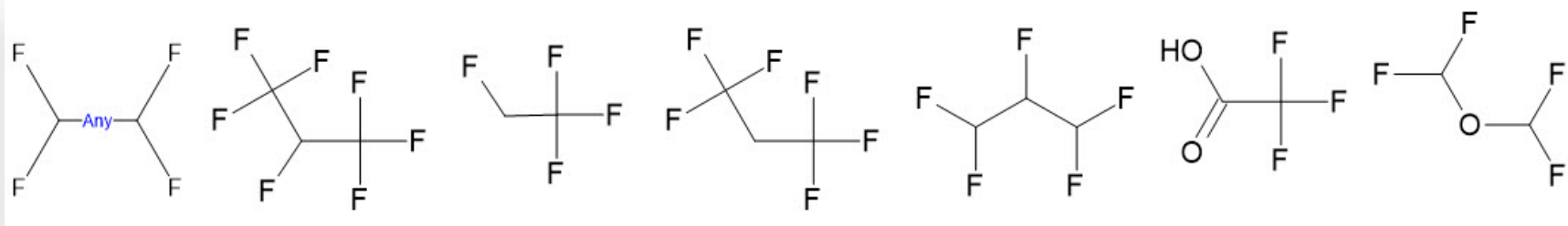
N-Methyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide
DTXSID: DTXSID7027831
PubChem: 24
CPDAT: 16

0 related chemical
structures with this



- What is a PFAS? Different definitions from different groups and publications.
- Difficult to get to a consistent definition
- We have taken an iterative approach
 - Substances with specific substructural elements as chemical “structures”

PFAS Structure List (8163)



EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

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

Search PFASSTRUCT Chemicals
☐ 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

Select all Download Send to Batch Search Name

8163 chemicals

DTXSID CASRN TOXCAS

Hide chemicals that are: Filter by Name or CASRN

(((Perfluorodecyl)ethylsulphonyl)methyl)oxirane
DTXSID:DTXSID70880957
CASRN:72276-05-2
TOXCAS:-

((2,2,3,3-Tetrafluoropropoxy)methyl)oxirane
DTXSID:DTXSID70880230
CASRN:19932-26-4
TOXCAS:-

((Perfluoro-11-methyldodecyl)ethyl) dihydroxyacetone
DTXSID:DTXSID60240985
CASRN:94200-57-4
TOXCAS:-

((Perfluoro-13-methyltetradecyl)ethyl) acrylate
DTXSID:DTXSID80238647
CASRN:91615-22-4
TOXCAS:-

Building a “Master PFAS List”

- What is a PFAS? Different definitions from different groups and publications.
- Difficult to get to a consistent definition
- We have taken an iterative approach
 - Substances with specific substructural elements as chemical “structures”
 - 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.

PFAS|EPA PFAS chemicals without explicit structures

 Search PFASDEV1 Chemicals

☐ 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 and filtering out chemical structures. This list remains under constant curation and expansion.

Number of Chemicals: 1097

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

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

1-Propene, 1,1,2,3,3,3-hexafluoro-, polymer with 1,1-difluoroethene, ethe...

149935-01-3 | DTXSID00108732

Searched by CAS-RN.

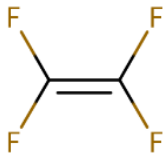
Select allDownloadSend to Batch SearchRelationshipCASRNDTXSIDTOXCASTHide chemicals that are:Filter by Name or CASRN

Searched Chemical

5 related chemical structures with this substance

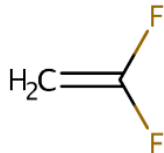
1-Propene, 1,1,2,3,3,3-hexafluoro-, poly...
CASRN:149935-01-3
DTXSID:DTXSID00108732
TOXCAST:-

Polymer




Tetrafluoroethylene
CASRN:116-14-3
DTXSID:DTXSID6021325
TOXCAST:-

Polymer



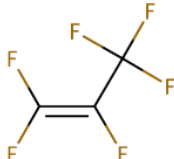
Vinylidene fluoride
CASRN:75-38-7
DTXSID:DTXSID3021439
TOXCAST:-

Polymer



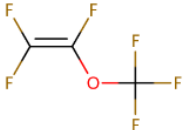
Ethylene
CASRN:74-85-1
DTXSID:DTXSID1026378
TOXCAST:-

Polymer



1,1,2,3,3,3-Hexafluoro-1-propene
CASRN:116-15-4
DTXSID:DTXSID2026949
TOXCAST:-

Polymer



Trifluoro(trifluoromethoxy)ethylene
CASRN:1187-93-5
DTXSID:DTXSID3051599
TOXCAST:-

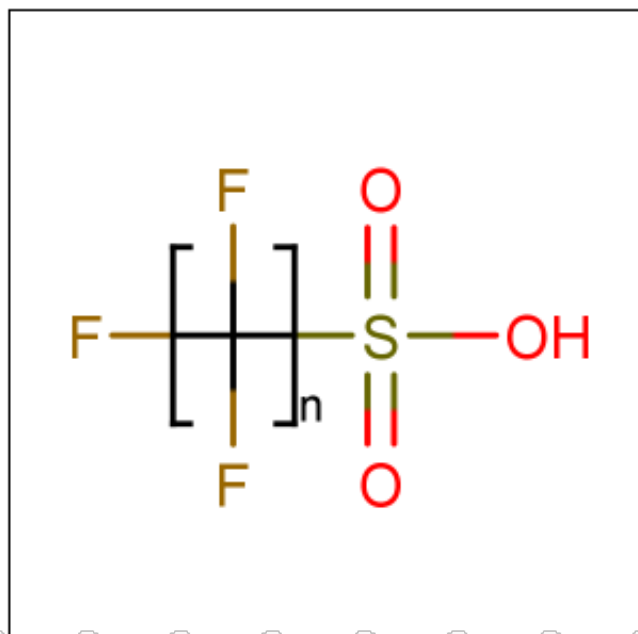
“Markush” Chemical Categories

- PFOS is a linear perfluoroalkyl sulfonate

Perfluoroalkyl sulfonates

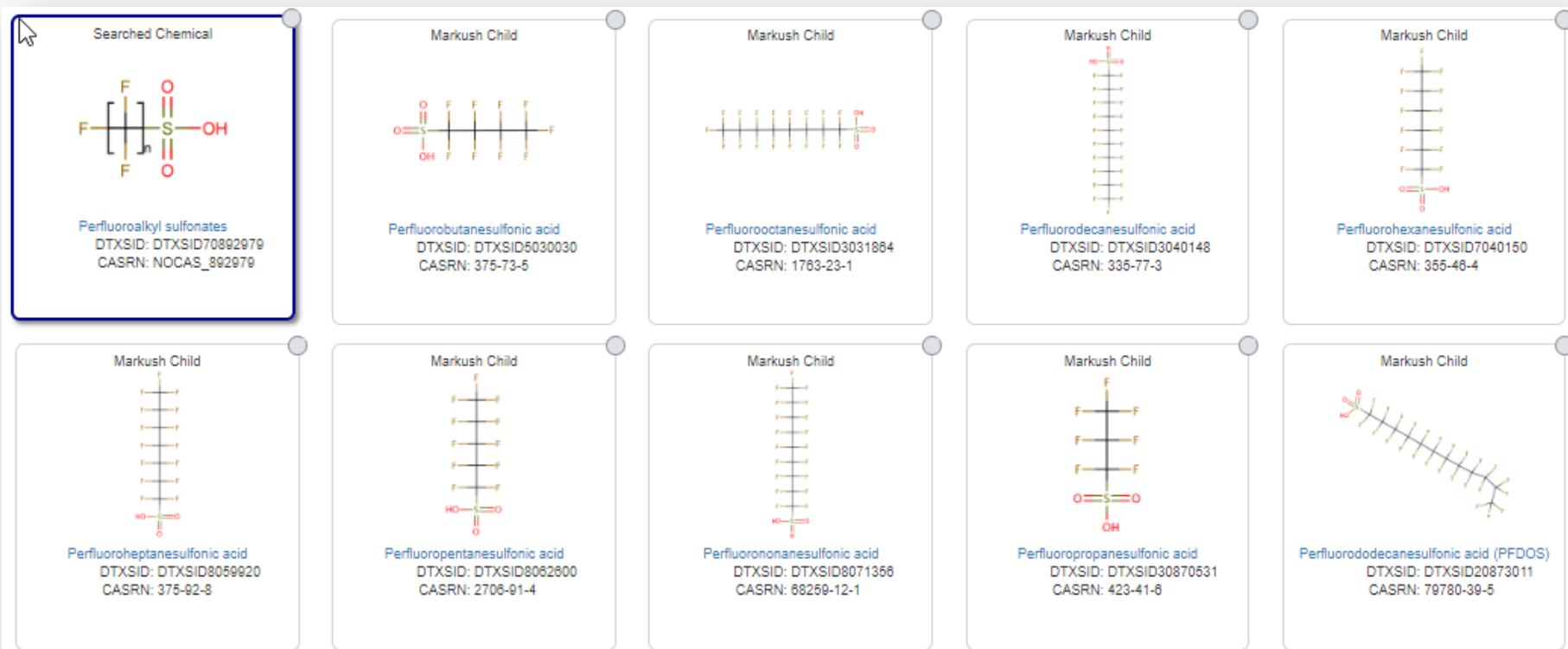
NOCAS_892979 | DTXSID70892979

Searched by DSSTox Substance Id.



...and their Markush Children...

- Linear perfluoroalkyl sulfonates has children...



PFAS Categories in Development

PFAS|EPA Structure-based Categories

☐ Identifier substring search

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

112 chemicals

Select all

Download

Send to Batch Search

Mono.Mass



CASRN



DTXSID



Hide chemicals that are:

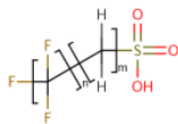
Filter by Name or CASRN



C4+ Perfluorinated chemicals

CASRN:NOCAS_1015355

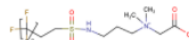
DTXSID:DTXSID401015355



Fluorotelomer (linear) sulfonic acids

CASRN:NOCAS_892558

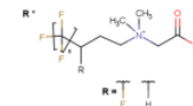
DTXSID:DTXSID50892558



Fluorotelomer Sulfonamido Betaines

CASRN:NOCAS_892972

DTXSID:DTXSID50892972



Fluorotelomer betaines


CASRN:NOCAS_892973

DTXSID:DTXSID10892973

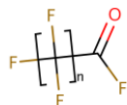
PFAS Categories in Development (112 categories so far...)

Vol. 127, No. 1 | Brief Communication

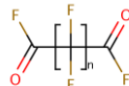
A Chemical Category-Based Prioritization Approach for Selecting 75 Per- and Polyfluoroalkyl Substances (PFAS) for Tiered Toxicity and Toxicokinetic Testing

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

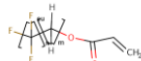
Published: 11 January 2019 | CID: 014501 | <https://doi.org/10.1289/EHP4555> | **Cited by:** 17



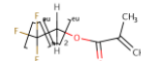
Perfluoroalkyl acyl fluorides
CASRN:NOCAS_893647
DTXSID:DTXSID10893647



Perfluoroalkyl symmetric diacyl fluorides
CASRN:NOCAS_893648
DTXSID:DTXSID70893648



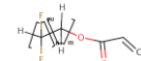
Fluorotelomer (linear) acrylates
CASRN:NOCAS_893800
DTXSID:DTXSID70893800



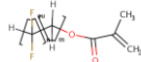
Fluorotelomer (linear) methacrylates
CASRN:NOCAS_893801
DTXSID:DTXSID30893801



Fluorotelomer (linear) n:2 alcohols
CASRN:NOCAS_893802
DTXSID:DTXSID90893802



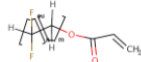
Fluorotelomer (linear) n:2 acrylates (-CH₂-)
CASRN:NOCAS_893803
DTXSID:DTXSID50893803



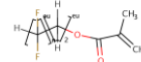
Fluorotelomer (linear) methacrylates (-C-)
CASRN:NOCAS_893804
DTXSID:DTXSID10893804



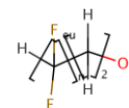
Fluorotelomer (linear) alcohols (-CHF₂)
CASRN:NOCAS_893805
DTXSID:DTXSID70893805



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



Fluorotelomer (linear) n:2 methacrylates ...
CASRN:NOCAS_893815
DTXSID:DTXSID20893815



Fluorotelomer (linear) n:2 alcohols (-CHF₂)
CASRN:NOCAS_893816
DTXSID:DTXSID80893816




Fluorotelomer (linear) n:2 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

 **United States
Environmental Protection
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

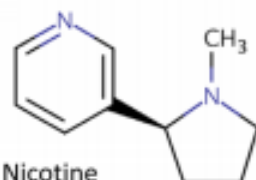
Presence in Lists:

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

SUPPORTING MASS SPECTROMETRY

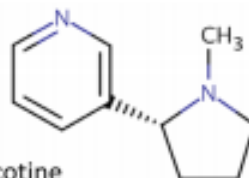
Open Science for Identifying “Known Unknown” Chemicals

Emma L. Schymanski^{*,†} and Antony J. Williams^{*,‡}



Nicotine

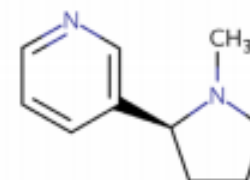
CN1CCC[C@H]1C1=CN=CC=C1
DTXSID1020930 | SNICXCGAKADSCV
54-11-5 | **162.1157** | 0.929 | **72**
Tox: **yes** | Expo: **yes** | Bioassay: **yes**



D-Nicotine

CN1CCC[C@H]1C1=CN=CC=C1
DTXSID004635 | SNICXCGAKADSCV
25162-00-9 | **162.1157** | 0.929 | **20**
Tox: **no** | Expo: **yes** | Bioassay: **yes**

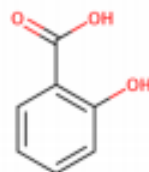
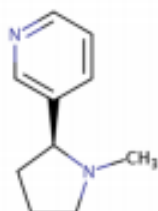
LEGEND: Name, SMILES
DTXSID | InChIKey 1st Block
CAS | Monoiso. Mass | logP | Sources
Data on: Toxicity | Exposure | Bioassays



HCl

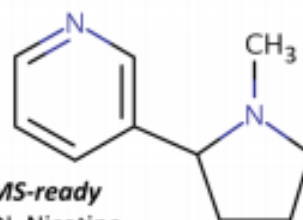
Nicotine hydrochloride

Cl.CN1CCC[C@H]1C1=CN=CC=C1
DTXSID602093 | HDJBTCJIMNXEW
2820-51-1 | **198.0924** | 0.929 | **9**
Tox: **no** | Expo: **yes** | Bioassay: **yes**



Benzoic acid, 2-hydroxy-, compd. with
3-[(2S)-1-methyl-2-pyrrolidinyl]pyridine (1:1)

OC(=O)C1=CC(=O)C=CC=C1.CN1CCC[C@H]1C1=CN=CC=C1
DTXSID5075319 | AIBWPBUAKCMKNS
29790-52-1 | **300.1474** | 0.929 | **6**
Tox: **no** | Expo: **yes** | Bioassay: **no**



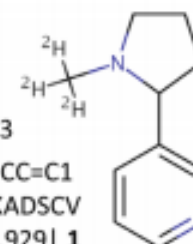
MS-ready

DL-Nicotine

CN1CCCC1C1=CN=CC=C1
DTXSID3048154 | SNICXCGAKADSCV
22083-74-5 | **162.1157** | 0.953 | **9**
Tox: **yes** | Expo: **no** | Bioassay: **yes**

DL-Nicotine-d3

[2H]C([2H])([2H])N1CCCC1C1=CN=CC=C1
DTXSID80442666 | SNICXCGAKADSCV
69980-24-1 | **165.1345** | 0.929 | **1**
Tox: **no** | Expo: **no** | Bioassay: **no**



Advanced Search


Supporting Target/Non-Target MS

Mass Search

[±](#) Min/Max


Adduct

All Adducts

Neutral 

☐ Choose adduct from dropdown

Mass


Da 

±



Error

Da

ppm


Search 

Molecular Formula Search


☐ MS Ready Formula ☒ Exact Formula 

Formula

C8HF17O3S

Search 

2 Chemicals match the formula

 United States
Environmental Protection
Agency

Home Advanced Search Batch Search Lists Predictions Downloads


Share Search all data

Search Results


Searched by Exact Molecular Formula: C₈H₁₇O₃S.

2 of 2 chemicals visible


Select all Download Send to Batch Search Default DTXSID PubChem CPDAT Multicomponent Chemicals Filter by Name or CASR



Perfluorooctanesulfonic acid
DTXSID: DTXSID3031864
PubChem: 68
CPDAT: 10



Heptadecafluorooctane-2-sulfonic acid
DTXSID: DTXSID30895921
PubChem: 0
CPDAT: 0

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 **Mass Search** 


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Search 

Molecular Formula Search 

☒ MS Ready Formula  ☐ Exact Formula 

Formula

C8HF17O3S

Search 

23 Chemicals match the formula

EPA United States Environmental Protection Agency

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Searched by MS Ready Formula: C₈HF₁₇O₃S.

23 chemicals

Select all Download Send to Batch Search Default DTXSID PubChem CPDAT

Hide chemicals that are: Filter by Name or CAS#

Chemical Name	DTXSID	PubChem	CPDAT
Perfluorooctanesulfonic acid	DTXSID03031864	68	10
Lithium perfluorooctanesulfonate	DTXSID02032421	32	14
Potassium perfluorooctanesulfonate	DTXSID08037706	59	18
Ammonium perfluorooctanesulfonate	DTXSID09067435	17	5
Tetraethylammonium perfluorooctanes...	DTXSID05069128	42	13
Bis(2-hydroxyethyl)ammonium perfluoro...	DTXSID02072049	19	4
Piperidinium perfluorooctanesulfonate	DTXSID00072352	4	0
Perfluorooctanesulfonate	DTXSID080108992	10	5
Tetrabutylammonium perfluorooctanes...	DTXSID040584995	14	0
Sodium perfluorooctanesulfonate	DTXSID050635462	13	0
Tetraethylammonium perfluorooctan...	DTXSID050881124	0	0
Magnesium heptadecafluorooctanesu...	DTXSID030881127	0	0

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

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DATABASE

Open Access

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



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