

US-EPA Comptox Chemicals Dashboard: an information hub for over five thousand per- & polyfluoroalkyl chemical substances

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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

*Spring 2019
ACS Spring Meeting, Orlando*

- **A publicly accessible website** delivering access:
 - ~875,000 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
 - Real time prediction of physchem and toxicity endpoints
 - **Over 5,000 of the chemicals are classed as PFAS Chemicals**

EPA activities around PFAS chemicals

<https://www.epa.gov/pfas>

Per- and Polyfluoroalkyl Substances (PFAS)

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What are PFAS?

PFAS is a category of man-made chemicals that are found in everyday items including food packaging, nonstick products, and stain repellent fabrics. [Learn more about PFAS](#), what they are, how people are exposed and [what EPA is doing](#).

1

2

3

"The [National Leadership Summit](#) on PFAS provided an unprecedented opportunity for stakeholders to share vital information and best practices regarding PFAS." -

Former Administrator Pruitt

- [Community Events](#)
- [Infographic](#)

Basic Information

- [What are PFAS?](#)
- [Why are PFAS important?](#)
- [How people are exposed?](#)

EPA Actions to Address PFAS


- [EPA actions](#)
- [National leadership summit and engagement](#)

Tools and Resources

- [EPA data and tools](#)
- [State information](#)
- [Site-specific resources](#)


CompTox Chemicals Dashboard

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

 EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists ▾ Predictions Downloads

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875 Thousand Chemicals

Chemicals

Product/Use Categories

Assay/Gene

☐ Identifier substring search

See what people are saying, read the dashboard [comments!](#)
Cite the Dashboard Publication [click here](#)


Latest News

[Read more news](#)

Journal of Cheminformatics article regarding "MS-Ready structures"

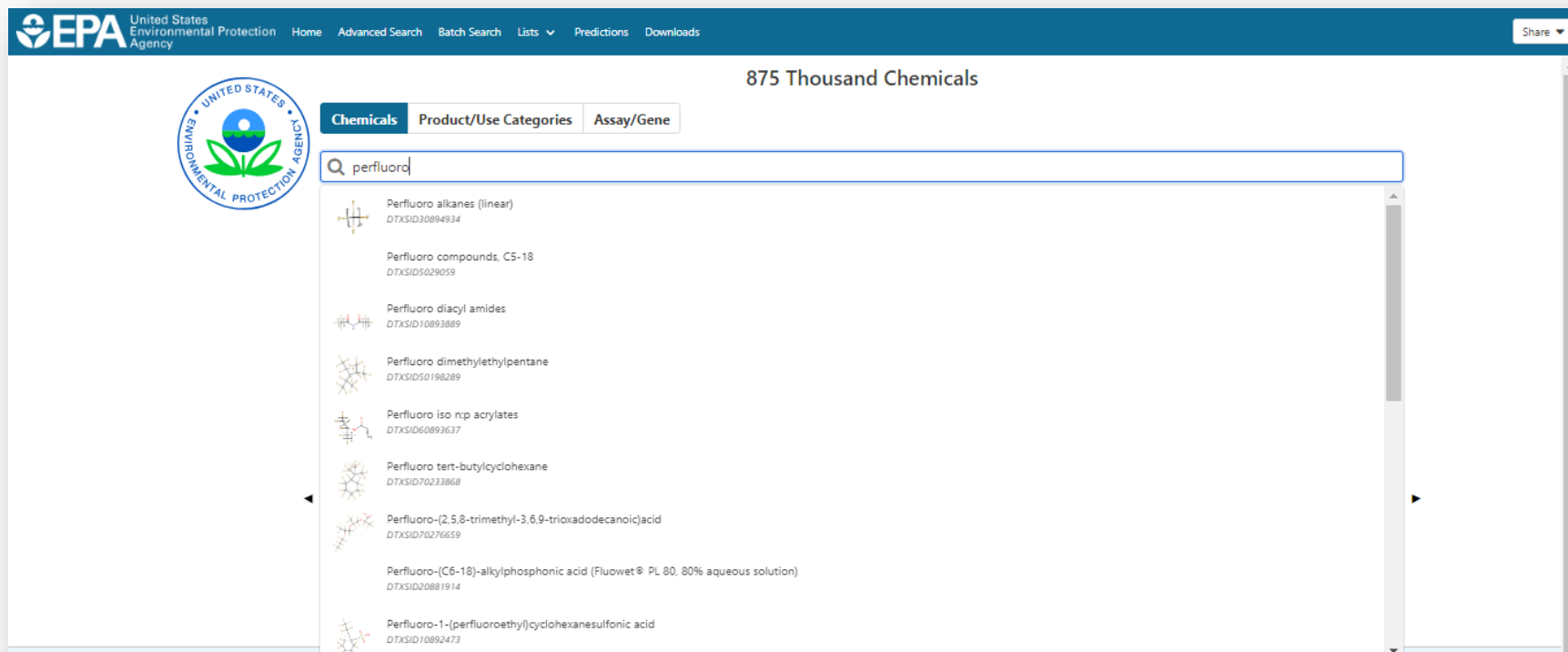
March 9th, 2019 at 1:09:45 PM

A recent article describes "MS-Ready structures", what they are, how they are generated and details regarding the benefits of these structures in navigating structure relationships across the dashboard. The article is published in the Journal of Cheminformatics [here](#).



CompTox Chemicals Dashboard


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



The screenshot shows 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 displays "875 Thousand Chemicals". Below this, there are tabs for "Chemicals", "Product/Use Categories", and "Assay/Gene". A search bar contains the text "perfluor". A list of chemical entries is displayed, 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

1 of ~875,000 Chemical Pages



United States
Environmental Protection
Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search all data

PFASListed in OECD Global Database

PFASEUOECD

DETAILS

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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

Executive Summary

PFASEUOECD

PFAS Listed in OECD Global
Database

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SYNONYMS

► LITERATURE

LINKS

COMMENTS

Reproductive Toxicology

✓ 13 Reproductive toxicity PODs available [↗](#)

Chronic Toxicology

✓ 15 Chronic toxicity PODs available [↗](#)

Subchronic Toxicology

✓ 1 Subchronic toxicity PODs available [↗](#)

Developmental Toxicology

✓ 8 Developmental toxicity PODs available [↗](#)

Acute Toxicology

✓ 65 Acute toxicity PODs available [↗](#)

Subacute Toxicology

✗ No subacute toxicity data available.

Neurotoxicology

✗ No neurotoxicology data available.

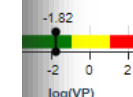
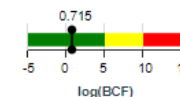
Endocrine System

✓ Endocrine Disruption Potential. Significant Estrogen Receptor activity seen. Chemical was positive in 5 ER assays (out of 17) and was positive in 2 AR assays (tested in 10) .

Submit Comment

Search all data

HEM PARAMETERS



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 ² K)

An automated curation procedure for addressing chemical errors and inconsistencies in public datasets used in QSAR modelling

K. Mansouri, C. M. Grulke, A. M. Richard, R. S. Judson & A. J. Williams

To cite this article: K. Mansouri, C. M. Grulke, A. M. Richard, R. S. Judson & A. J. Williams (2016)

An automate
datasets use
DOI: [10.1081](https://doi.org/10.1081)

Mansouri et al. *J Cheminform* (2018) 10:10
<https://doi.org/10.1186/s13321-018-0263-1>

To link to th

 Journal of Cheminformatics

RESEARCH ARTICLE

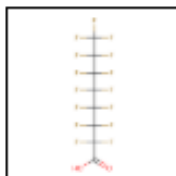
Open Access



OPERA models for predicting physicochemical properties and environmental fate endpoints

Kamel Mansouri^{1,2,3*} , Chris M. Grulke¹, Richard S. Judson¹ and Antony J. Williams¹

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	

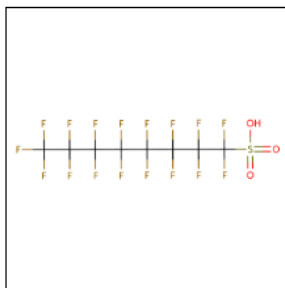
Detailed OPERA Prediction Reports

OPERA Models: Vapor Pressure

Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Print PDF



Model Results

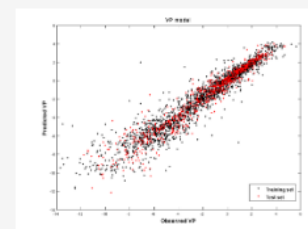
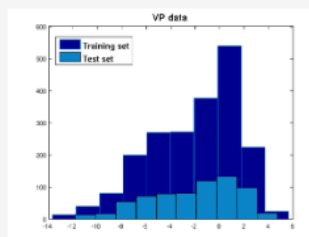
Predicted values: 1.49e-2 mmHg

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



N-Ethylperfluorooctanesulfonamide
Measured: 4.27957e-7
Predicted: 0.00000157466



Perfluorooctanesulfonamide
Measured: 0.248028
Predicted: 0.181011




Perfluorooctanoic acid
Measured: 0.525049
Predicted: 0.339896



Perfluorooheptanoic acid
Measured: 0.133015
Predicted: 0.127572

- Physicochemical property and environmental fate and transport data has been extracted from the literature
- OPERA models have been rebuilt with these data for new predictions
- Dramatic improvements in predictions for physchem endpoints – logP, AqSol, VP

Hazard Data – Human and Eco

 United States
Environmental Protection
Agency

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DETAILS

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ADME

► EXPOSURE

► BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES


SYNONYMS

► LITERATURE

LINKS

COMMENTS

DataType









 Ecotox Effect Level ▼

Download ▼

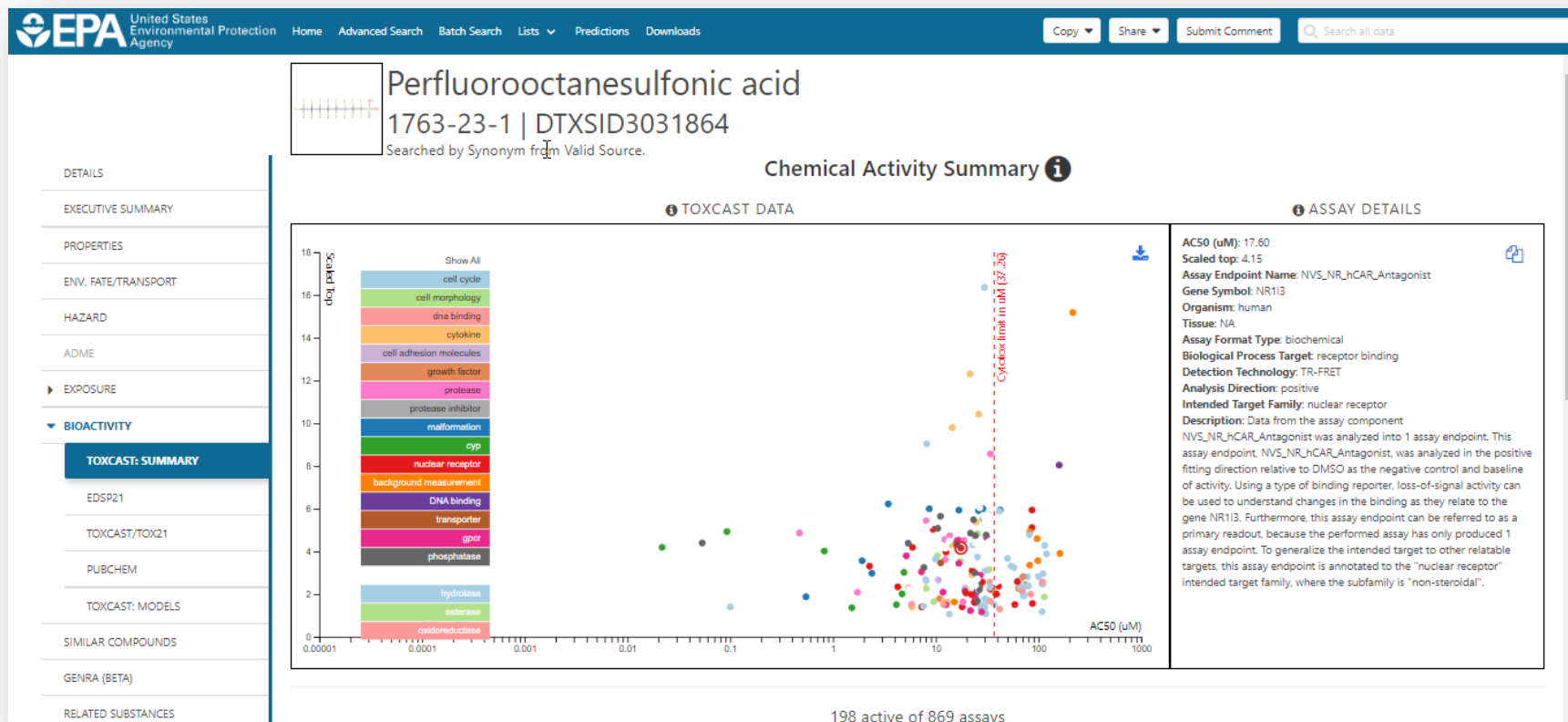
Human

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

- ToxVal Database contains following data:
 - ~30,000 chemicals
 - ~750,000 toxicity values
 - ~30 sources of data
 - ~21,000 sub-sources
 - ~4500 journals cited
 - ~70,000 literature citations



What is PFOS Called?

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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 CAS-RN**

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

Submit Comment

Search all data

Search query

↕

Quality

↕

Valid

Valid

Valid

Valid

Valid

Valid

Valid

Valid

Valid

Valid

Good

Other

Other

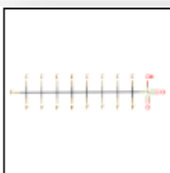
Other

Other

Other

Other

Other




Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by Synonym from Valid Source.

Abstract Sifter

1) Select PubMed starting point query then 2) click on Retrieve. 

Select a Query Term



Retrieve Articles

Select a Query Term

- Hazard
- Fate and Transport
- Metabolism/PK/PD
- Chemical Properties
- Exposure
- Mixtures
- Male Reproduction
- Androgen Disruption
- Female Reproduction
- GeneTox
- Cancer
- Clinical Trials
- Embryo and embryonic development
- Child (infant through adolescent)
- Dust and Exposure
- Food and Exposure
- Water and Exposure
- Algae
- Disaster / Emergency

Optionally, edit the query before retrieving.

"1763-23-1" OR "Perfluorooctanesulfonic acid" OR "perfluorooctane sulfonic acid"

Literature Searching - PubMed

Abstract Sifter

1) Select PubMed starting point query then 2) click on Retrieve.

Hazard [Retrieve Articles](#)

24 of 24 articles loaded...

Optionally, edit the query before retrieving.

("1763-23-1" OR "Perfluorooctanesulfonic acid" OR "perfluorooctane sulfonic acid") AND (NOAEL or NOEL OR LOEL or Rfd OR "reference dose" OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])

To find articles quickly, enter terms to sift abstracts.

exposure RfD immunotox [Clear Terms](#)

[Download / Send to...](#) [Download Sifter for Excel](#)

<input type="checkbox"/>	exposure	RfD	immunotox	Total	PMID	Year	Title	Authors	Journal	Rev
<input type="checkbox"/>	2	2	0	4	30798190	2019	Using 2003-2014 U.S. NHANES data to determine t...	Dong; Wang; Yu; Li; Naidu; Liu	Ecotoxicology and environmental safety	
<input type="checkbox"/>	8	0	0	8	29525662	2018	Modeling avian exposures to perfluoroalkyl substan...	Larson; Conder; Arblaster	Chemosphere	
<input type="checkbox"/>	2	5	1	8	28521193	2017	Issues raised by the reference doses for perfluoro...	Dong; Bahar; Jit; Kennedy; Priestly; Ng; Lamb; Liu; ...	Environment international	
<input type="checkbox"/>	0	0	0	0	24046276	2013	Dosimetric anchoring of in vivo and in vitro studies f...	Wambaugh; Setzer; Pitruzzello; Liu; Reif; Kleinstreu...	Toxicological sciences : an official journal of the So...	
<input type="checkbox"/>	0	0	0	0	22441698	2012	Perfluorooctane sulfonate increases β -oxidation of ...	Nordén; Westman; Venizelos; Engwall	Environmental science and pollution research inter...	
<input type="checkbox"/>	0	0	0	0	21467747	2011	Induction of apoptosis and CYP4A1 expression in S...	Kim; Jun Kwack; Sik Han; Seok Kang; Hee Kim; Yo...	The Journal of toxicological sciences	
<input type="checkbox"/>	0	0	0	0	21207445	2011	Aquatic predicted no-effect-concentration derivation...	Qi; Wang; Mu; Wang	Environmental toxicology and chemistry	
<input type="checkbox"/>	0	0	0	0	20879709	2010	Distribution of perfluorooctane sulfonate and other ...	Wang; Fu; Wang; Liang; Pan; Cai; Jiang	Environmental science & technology	
<input type="checkbox"/>	1	0	0	1	20709355	2010	Brominated flame retardants and perfluorinated co...	D'Hollander; Roosens; Covaci; Cornelis; Reynders; ...	Chemosphere	
<input type="checkbox"/>	2	0	0	2	19569327	2009	Perfluoroalkyl contaminants in an Arctic marine foo...	Kelly; Ikonou; Blair; Surridge; Hoover; Grace; G...	Environmental science & technology	
<input type="checkbox"/>	3	0	1	4	19343326	2009	Chronic effects of perfluorooctanesulfonate exposur...	Dong; Zhang; Zheng; Liu; Jin; He	Archives of toxicology	
<input type="checkbox"/>	3	0	0	3	19162172	2009	Gestational and lactational exposure to potassium ...	Butenhoff; Ehresman; Chang; Parker; Stump	Reproductive toxicology (Elmsford, N.Y.)	
<input type="checkbox"/>	2	0	0	2	19110351	2008	Behaviour of damselfly larvae (Enallagma cyathiger...	Van Gossum; Bots; Snijders; Meyer; Van Wassenb...	Environmental pollution (Barking, Essex : 1987)	
<input type="checkbox"/>	0	0	0	0	18754515	2008	Perfluoroalkyl acids in the egg yolk of birds from La...	Yoo; Kannan; Kim; Lee; Newsted; Giesy	Environmental science & technology	

Generalized Read-Across (GenRA)

EPA United States Environmental Protection Agency

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PFAS EUCED
PFAS Listed in OECD Global Database

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

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Step One: Analog Identification and Evaluation

Neighbors by: Chem: Morgan Fgrpts Filter by: invivo data

PFOS

PFOS-K Sulfonamid PFBS-K PFOA, ammon... PFHxA Sodium perfluor... Sulfuryl fluoride

Aldoxycarb Tetrakis(hydroxy... Bis(trichloromet...

of Analogs 10

Next

Summary Data Step Analogs

Substance	Invivo	Invivo	Invivo	Invivo	Invivo
PFOS	1	1	1	1	1
PFOS-K	1	1	1	1	1
Sulfonamid	1	1	1	1	1
PFBS-K	1	1	1	1	1
PFOA, ammon...	1	1	1	1	1
PFHxA	1	1	1	1	1
Sodium perfluor...	1	1	1	1	1
Sulfuryl fluoride	1	1	1	1	1
Aldoxycarb	1	1	1	1	1
Tetrakis(hydroxy...	1	1	1	1	1
Bis(trichloromet...	1	1	1	1	1

PFOS

PFOS-K

Sulfonamid

PFBS-K

PFOA, ammon...

PFHxA

Sodium perfluor...

Sulfuryl fluoride

Aldoxycarb

Tetrakis(hydroxy...

Bis(trichloromet...

Select and Review Analogs

Generalized Read-Across (GenRA)

EPA United States Environmental Protection Agency

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PFAS EUCED
PFAS Listed in OECD Global Database

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Step Two: Data Gap Analysis & Generate Data Matrix

Neighbors by: Chem: Morgan Fgprts Filter by: invivo data Summary Data Gap Analysis Group: ToxRef By: Tox Fingerprint Generate Data Matrix

Chemical Structure Diagram: A central PFOS molecule is surrounded by 10 analogs: Aldoxycarb, Tetrakis(hydroxy...), Bis(trichloromet...), Sulfuryl fluoride, Sodium perfluor..., PFHxA, PFOA, ammoni..., PFBS-K, Sulfuramid, and PFOS-K.

Summary Data Gap Analysis Table:

	bio_b21	bio_tox	chem_ct	tox_bcf
PFOS	31	821	21	95
PFOS-K	38	714	21	307
Sulfuramid	29	714	21	282
PFBS-K	2	714	19	187
PFOA, ammonium salt	19	714	20	345
PFHxA	24	714	17	85
Sodium perfluorohexano...	0	0	18	282
Sulfuryl fluoride	0	0	8	345
Bis(trichloromethyl)sulfone	0	0	8	158
Tetrakis(hydroxymethyl)...	25	0	8	408
Aldoxycarb	9	228	6	83

Generate Data Matrix Table:

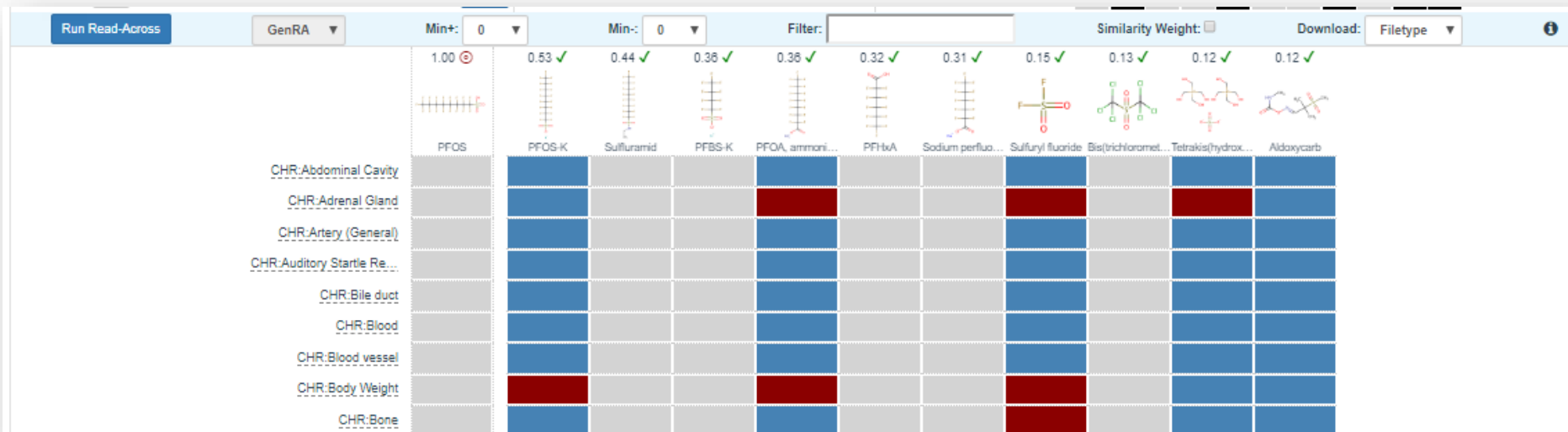
	PFOS	PFOS-K	Sulfuramid	PFBS-K	PFOA, ammonium	PFHxA	Sodium perfluorohexano...	Sulfuryl fluoride	Bis(trichloromethyl)sulfone	Tetrakis(hydroxymethyl)sulfone	Aldoxycarb
CHR:Abdominal Cavity											
CHR:Adrenal Gland											
CHR:Artery (General)											
CHR:Auditory Stairle Re...											
CHR:Bile duct											
CHR:Blood											
CHR:Blood vessel											
CHR:Body Weight											
CHR:Bone											
CHR:Bone Marrow											
CHR:Brain											
CHR:Bronchus											

Select and Review Analogs

Review Available Data


Fingerprint indicating available data

Generalized Read-Across (GenRA)



Red : Toxicity effects.
Blue: No Toxicity effects
Grey : Absence of data

Are there Similar Compounds?

 United States Environmental Protection Agency

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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.

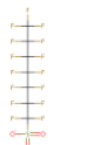
Searched with a similarity threshold of 0.8

83 chemicals

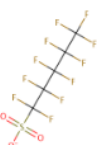
Select all Download Send to Batch Search Similarity DTXSID CASRN TOXCAST Similarity Hide chemicals that are: Filter by Name or CASRN




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



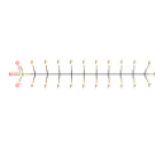
Perfluoropentanesulfonate
DTXSID: DTXSID70892479
CASRN: 175905-36-9
TOXCAST: -
Similarity: 1.00



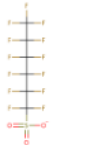
Magnesium bis(heptadecafluorooctanes...
DTXSID: DTXSID60881314
CASRN: 91036-71-4
TOXCAST: -
Similarity: 1.00



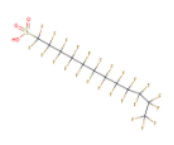
Perfluorobutanesulfonate
DTXSID: DTXSID60873015
CASRN: 45187-15-3
TOXCAST: -
Similarity: 1.00




Perfluorododecane-1-sulfonic acid



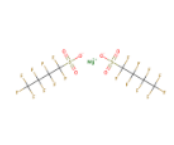
Perfluorobutanesulfonate



Perfluorododecane-1-sulfonic acid



Perfluoropentane-1-sulfonic acid



Magnesium nonafluorobutanesulfonate

Relationships in the data

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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 CASRN

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 perfluorooctanes...	DTXSID: DTXSID5069128	PubChem: 42	

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

Perfluorooctanesulfonic acid
DTXSID: DTXSID3031864
PubChem: 68
CPDAT: 10

Lithium perfluorooctanesulfonate
DTXSID: DTXSID2032421
PubChem: 32
CPDAT: 14

Potassium perfluorooctanesulfonate
DTXSID: DTXSID8037706
PubChem: 59
CPDAT: 18

Ammonium perfluorooctanesulfonate
DTXSID: DTXSID9067435
PubChem: 17
CPDAT: 5

Bis(2-hydroxyethyl)ammonium perfluorooctanesulfonate
DTXSID: DTXSID2072049
PubChem: 19
CPDAT: 4

Perfluorooctanesulfonate
DTXSID: DTXSID80108992
PubChem: 10
CPDAT: 5

Sodium perfluorooctanesulfonate
DTXSID: DTXSID50635462
PubChem: 13
CPDAT: 0

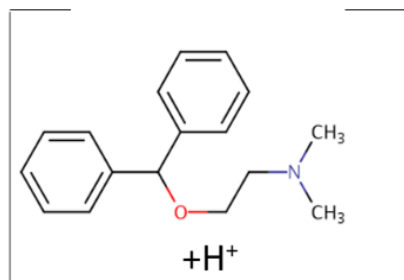
Heptadecafluorooctane-1-ylsulfonic acid
DTXSID: DTXSID00892720
PubChem: 0
CPDAT: 0

heptaecafluoro(1,2,3,4-13C4)octane-1-ylsulfonic acid
DTXSID: DTXSID80894101
PubChem: 0
CPDAT: 0

Using data relationships

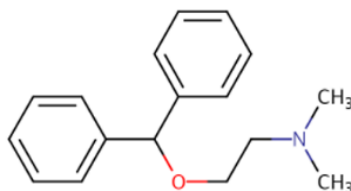
- We have purposely built relationships in the data. Specifically, “MS-Ready mappings”

A) Molecular Ion



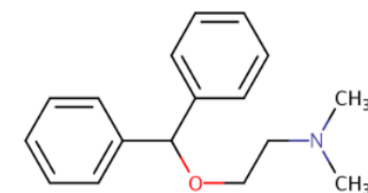
$m/z \approx 256.1702$

B) MS-Ready Form

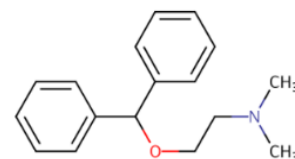


monoisotopic mass= 255.1623
 $C_{17}H_{21}NO$
DTXCID802949

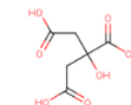
C) Mappings from MS-Ready



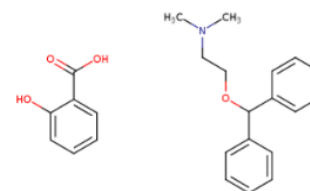
Diphenhydramine
 $C_{17}H_{21}NO$ | 255.1623
DTXSID4022949



Diphenhydramine
hydrochloride
 $C_{17}H_{22}ClNO$ | 291.1390
DTXSID4020537



Diphenhydramine citrate
 $C_{23}H_{29}NO_8$ | 447.1893
DTXSID80237211



Diphenhydramine salicylate
 $C_{24}H_{27}NO_4$ | 393.1940
DTXSID10225883

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

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Search Results


Searched by Exact Molecular Formula: C₈HF₁₇O₃S.

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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Advanced Search




Supporting Target/Non-Target MS


 **Mass Search** 


± Min/Max



Adduct All Adducts

Neutral   Choose adduct from dropdown

Mass   Error  ppm


Search 

Molecular Formula Search 

☒ MS Ready Formula  ☐ Exact Formula 

Formula

C8HF17O3S

Search 

23 Chemicals match the formula

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Search Results

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	PubChem: 68	CPDAT: 10
Lithium perfluorooctanesulfonate	DTXSID2032421	PubChem: 32	CPDAT: 14
Potassium perfluorooctanesulfonate	DTXSID08037706	PubChem: 59	CPDAT: 18
Ammonium perfluorooctanesulfonate	DTXSID9067435	PubChem: 17	CPDAT: 5
Tetraethylammonium perfluorooctanes...	DTXSID5069128	PubChem: 42	CPDAT: 13
Bis(2-hydroxyethyl)ammonium perfluoro...	DTXSID2072049	PubChem: 19	CPDAT: 4
Piperidinium perfluorooctanesulfonate	DTXSID0072352	PubChem: 4	CPDAT: 0
Perfluorooctanesulfonate	DTXSID80108992	PubChem: 10	CPDAT: 5
Tetrabutylammonium perfluorooctanesu...	DTXSID40584995	PubChem: 14	CPDAT: 0
Sodium perfluorooctanesulfonate	DTXSID50635462	PubChem: 13	CPDAT: 0
Tetraethylammonium perfluorooctanesu...	DTXSID50881124	PubChem: 0	CPDAT: 0
Magnesium heptafluorooctanesulfonate	DTXSID30881127	PubChem: 0	CPDAT: 0

23 Chemicals match the formula

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Search Results


Searched by MS Ready Formula: C₈HF₁₇O₃S.

23 chemicals

Select all Download Send to Batch Search Default Filter by Name or CASRN

Structure	DTXSID	Preferred Name	CASRN	QC Level	CPDat Count	Number of Sources	PubChem Data Sources	PubMed Ref. Counts	Monoisotopic Mass
	DTXSID031864 ToxCast™	Perfluorooctanesulfonic acid	1763-23-1	Level 1	10	109	68	1124	499.937494
	DTXSID2032421 ToxCast™	Lithium perfluorooctanesulfonate	29457-72-5	Level 1	14	41	32	0	505.945672
	DTXSID8037706 ToxCast™	Potassium perfluorooctanesulfonate	2795-39-3	Level 1	18	63	59	0	537.893375
	DTXSID9067435	Ammonium perfluorooctanesulfonate	29081-56-9	Level 1	5	21	17	0	516.964043
	DTXSID5069128	Tetraethylammonium perfluorooctanesulfonate	56773-42-3	Level 2	13	32	42	0	629.089243

Batch Searches

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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

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

Display All Chemicals

Download Chemical Data

Select Output Format:
Excel

Download


Customize Results

- ☐ Select All
- ☐ Select All in Lists

Presence in Lists:

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

Batch Searches

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

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

Step Six: Click "Download"

Select Output Format:
Excel

Download

Customize Results

- ☐ Select All
- ☐ Select All in Lists

Chemical Identifiers

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

Structures

- ☐ Mol File
- ☐ SMILES
- ☐ InChI String
- ☒ MS-Ready SMILES
- ☐ QSAR-Ready SMILES

Intrinsic And Predicted Properties

- ☐ Molecular Formula
- ☐ Average Mass
- ☐ Monoisotopic Mass
- ☒ TEST Model Predictions
- ☒ OPERA Model Predictions

Metadata


Presence in Lists:

- ☐ 40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities
- ☐ AEGLs: Acute Exposure Guideline Levels
- ☐ ANDROGEN: Androgen Receptor Chemicals
- ☐ ARTICLE: Bench-Mark Dose Human Health Assessment List (Wignall et al., 2014)
- ☐ ATSDR: Minimal Risk Levels (MRLs) for Hazardous Substances
- ☐ ATSDR: Toxic Substances Portal Chemical List
- ☐ California Office of Environmental Health Hazard Assessment
- ☐ CERAPP: Collaborative Estrogen Receptor Activity Prediction Project
- ☐ CHEMINV: ToxCast/Tox21 Chemical inventory available as DMSO solutions (20181123)
- ☐ CHEMINV: EPA Chemical Inventory for ToxCast
- ☐ CHEMINV: EPA ToxCast CHEMINV list of volatiles
- ☐ CHEMINV: EPA ToxCast Cheminventory chemicals with stability problems
- ☐ CHEMINV: EPA ToxCast Cheminventory DMSO Insolubles
- ☐ CHEMINV: EPA ToxCast Cheminventory List of Reactives
- ☐ DRUGS: DrugBank database from the University of Alberta
- ☐ DRUGS: ITNANTIBIOTIC list of antibiotics
- ☐ DRUGS: Pharmaceutical List with EU, Swiss, US Consumption Data
- ☐ DRUGS: Statin drugs
- ☐ ECOTOX: Ecotoxicology knowledgebase
- ☐ Endocrine Disruptor Screening Program (EDSP) Universe of Chemicals
- ☐ ENDOCRINE: EDSR21 Tier 1 Screening Chemicals List 1

- Specific subsets of chemicals, “lists”, can be displayed on the dashboard
- If there are chemicals that map together then these link to existing:
 - Property data
 - Hazard data
 - Exposure data
 - *In vitro* bioassay data
 - Documents and Literature

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

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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/>

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

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Default



DTXSID

PubChem

CPDAT

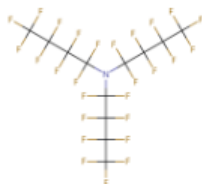


Hide chemicals that are:

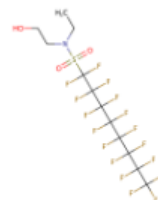
Filter by Name or CASRN



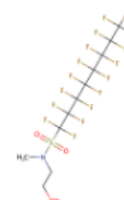
Perfluorooctanesulfonyl fluoride
DTXSID: DTXSID5027140
PubChem: 71
CPDAT: 6



Perfluorotributylamine
DTXSID: DTXSID0027141
PubChem: 71
CPDAT: 0

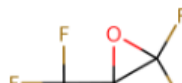


N-Ethyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide
DTXSID: DTXSID6027426
PubChem: 54
CPDAT: 3



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

0 related chemical
structures with this



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.

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

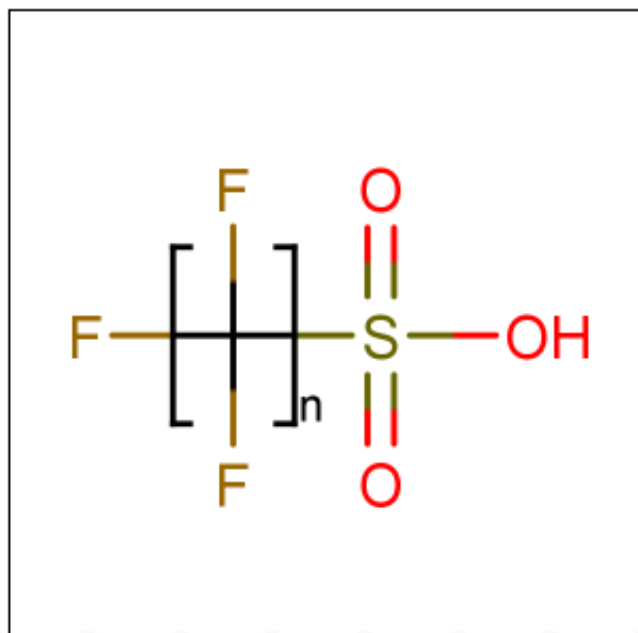
↓ 1-Propene, 1,1,2,3,3,3-hexafluoro-, polymer with 1,1-difluoroethene, ethene, 1,1,2,2-tetrafluoroethene and 1,1,2-trifluoro-2-(trifluoromethoxy)ethene
149935-01-3 | DTXSID00108732

- PFOS is a member of linear perfluoroalkyl sulfonates

Perfluoroalkyl sulfonates

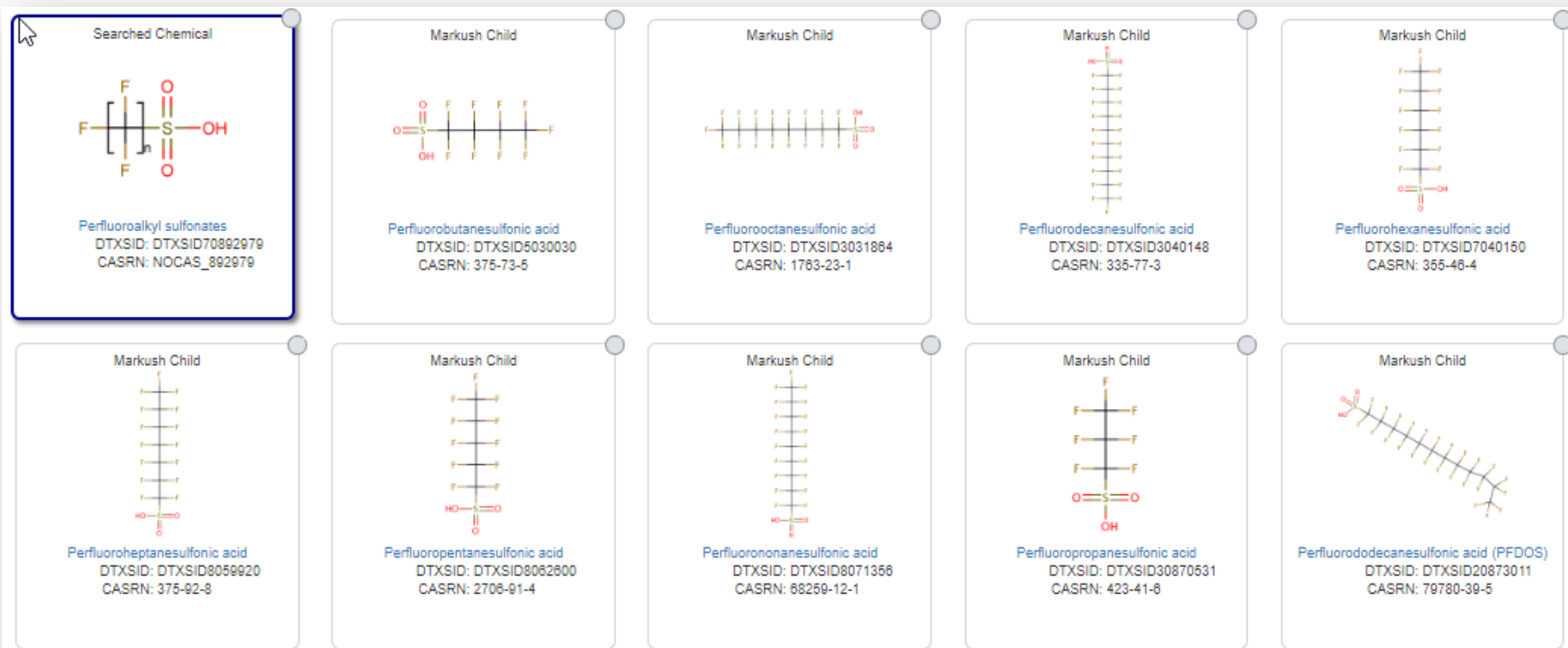
NOCAS_892979 | DTXSID70892979

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

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Default



DTXSID

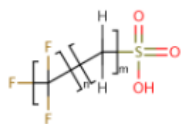
PubChem

CPDAT



Hide chemicals that are:

Filter by Name or CASRN



Fluorotelomer (linear) sulfonic acids

DTXSID: DTXSID50892558

PubChem: 0

CPDAT: 0

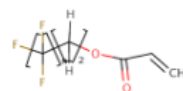


Fluorotelomer (linear) alcohols

DTXSID: DTXSID10893581

PubChem: 0

CPDAT: 0

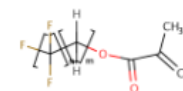


Fluorotelomer (linear) n:2 acrylates

DTXSID: DTXSID70893582

PubChem: 0

CPDAT: 0



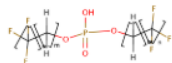
Fluorotelomer (linear) n:2 methacrylates

DTXSID: DTXSID30893583

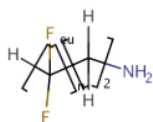
PubChem: 0

CPDAT: 0

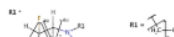
PFAS Categories in Development



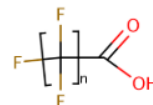
Fluorotelomer (linear) phosphate esters...



Fluorotelomer (linear) n:2 amines (prim...



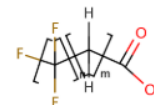
Fluorotelomer (linear) amines (tertiary) (...)



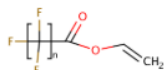
Perfluoroalkyl (linear) carboxylic acids



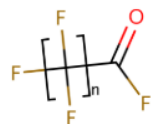
Fluorotelomer (linear) alcohols



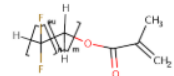
Fluorotelomer (linear) carboxylic acids



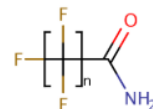
Perfluoroalkyl esters (vinyl)



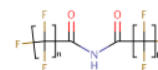
Perfluoroalkyl acyl fluorides



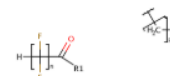
Fluorotelomer (linear) methacrylates (-...



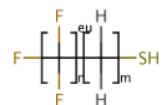
Perfluoroalkyl (linear) amides (primary)



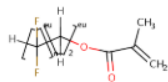
Perfluoro diacyl amides



Polyfluoroalkyl (linear) (-CF2H) alkyl (lin...



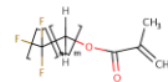
Fluorotelomer (linear) thiols



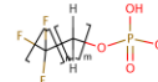
Fluorotelomer (linear) n:2 methacrylate...



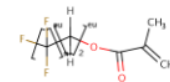
Perfluoroalkyl amidines



Fluorotelomer (linear) n:2 methacrylates

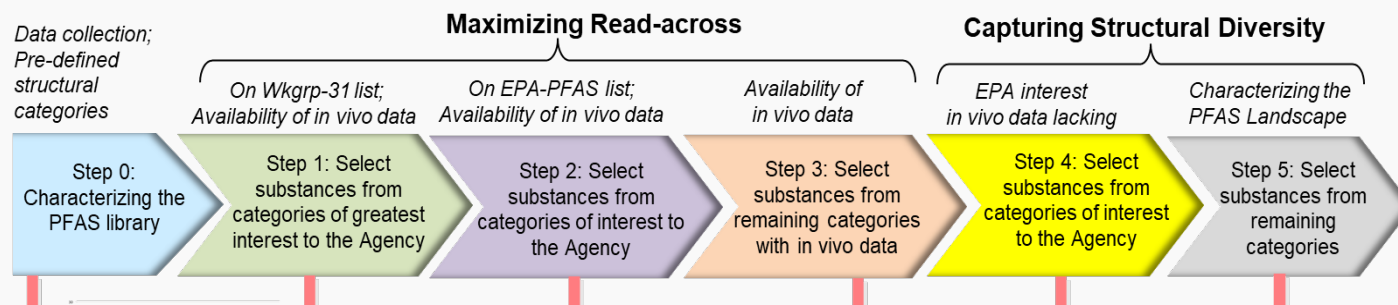


Fluorotelomer (linear) phosphate esters...



Fluorotelomer (linear) methacrylates

- Development of a high-throughput screening library and collection of physical samples (~430)
- **150** PFAS for screening based on categories, diversity, exposure considerations, procurability and testability, availability of existing toxicity data



Brief Communication

A Section 508–conformant HTML version of this article is available at <https://doi.org/10.1289/EHP4555>.

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

Grace Patlewicz,¹ Ann M. Richard,¹ Antony J. Williams,¹ Christopher M. Grulke,¹ Reeder Sams,¹ Jason Lambert,² Pamela D. Noyes,³ Michael J. DeVito,⁴ Ronald N. Hines,⁵ Mark Strynar,⁶ Annette Guiseppi-Elie,⁶ and Russell S. Thomas¹

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. (**OPERA 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
 - Physical library of 100s of chemicals has been acquired
 - High-throughput screening of ~150 chemicals
 - Classification approaches and Markush representations

- Dashboard development team
- Database curation team
- NERL – Jon Sobus, Elin Ulrich and Mark Strynar

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