

# NORMAN Suspects meet the US EPA CompTox Chemistry Dashboard

**Emma Schymanski**, Eawag: Swiss Federal Institute of Aquatic Science and Technology  
**Antony J. Williams & Andrew McEachran**, United States Environmental Protection Agency



Chemistry Dashboard

Search a chemical by systematic name, synonym, CAS number, or InChIKey



# What is the CompTox Chemistry Dashboard?

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

## Aims of US EPA's Computational Toxicity Program:

- Integrate advances in biology, chemistry, and computer science to...
- Prioritize chemicals based on potential human and ecological health risks

## The CompTox Chemistry Dashboard:

- Provides access to ~747,000 chemical substances & associated data
- Years of investment/experience in data validation and curation
- Data include: (plus a LOT more ...)
  - Experimental and predicted physicochemical properties
  - ToxCast bioassay screening data
  - Product and functional use information and more
- Search capabilities include:
  - Mass or formula-based searching
  - Rank-ordering of results via functional use statistics to prioritize chemicals

# The Dashboard in brief

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



## Chemistry Dashboard

Search a chemical by systematic name, synonym, CAS number, or InChIKey



Single component search  Ignore isotopes

See what people are saying, read the dashboard [comments!](#)

Need more? Use [advanced search](#).

747 Thousand Chemicals

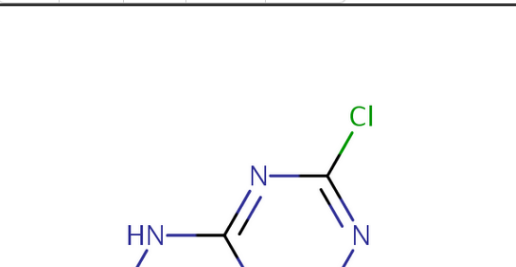
# The Dashboard in brief

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

Atrazine

1912:24-9|DTXSID9020112

© Searched by Approved Name: Found 1 result for 'atrazine'.



Summary

- LogP: Octanol-Water
- Water Solubility
- Density
- Melting Point
- Boiling Point
- Surface Tension
- Vapor Pressure
- LogKoa: Octanol-Air
- Henry's Law
- Index of Refraction
- Molar Refractivity

Chemical Properties

Comments

## Wikipedia

Atrazine is an herbicide of the triazine class. Atrazine is used to prevent pre- and postemergence broadleaf weeds in crops such as maize (corn) and sugarcane and on turf, such as golf courses and residential lawns. It is one of the most widely used herbicides in US and Australian agriculture. It was banned in the European Union in October 2003, when the EU found groundwater levels exceeding the limits set by regulators, and Syngenta could neither show that this could be prevented nor that... [Read more](#)

Download as:

Property	Average		Median		Range		Unit
	Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
LogP: Octanol-Water	2.61 (1)	2.76 (4)	2.61	2.76	2.61	2.50 to 3.05	-
Water Solubility	1.30e-04 (1)	1.46e-02 (4)	1.30e-04	1.46e-02	1.30e-04	1.50e-04 to 5.71e-02	mol/L
Density	-	1.27 (1)	-	1.27	-	-	g/cm <sup>3</sup>
Melting Point	174 (6)	151 (3)	175	151	173 to 177	114 to 185	°C
Boiling Point	-	312 (3)	-	312	-	284 to 339	°C
Surface Tension	-	53.8 (1)	-	53.8	-	-	dyn/cm
Vapor Pressure	7.21e-11 (1)	4.47e-06 (3)	7.21e-11	4.47e-06	7.21e-11	2.06e-07 to 1.27e-05	mmHg
LogKoa: Octanol-Air	-	8.38 (1)	-	8.38	-	-	-
Henry's Law	-	4.20e-10 (1)	-	4.20e-10	-	-	atm-m <sup>3</sup> /mole
Index of Refraction	-	1.61 (1)	-	1.61	-	-	-
Molar Refractivity	-	58.5 (1)	-	58.5	-	-	cm <sup>3</sup>
pKa Basic Apparent	-	2.27 (1)	-	2.27	-	-	-

Literature

# The Dashboard in brief

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

## Atrazine

1912-24-9|DTXSID9020112

© Searched by Approved Name: Found 1 result for 'atrazine'.



Wikipedia

Atrazine is an herbicide of the triazine class. Atrazine is used to prevent pre- and postemergence broadleaf weeds in crops such as maize (corn) and sugarcane and on turf, such as golf courses and residential lawns. It is one of the most widely used herbicides in US and Australian agriculture. It was banned in the European Union in October 2002, when the EU found groundwater levels

- Chemical Properties
- Env. Fate/Transport
- Synonyms
- External Links
- Toxicity Values (Beta)
- Exposure
- Bioassays
- Similar Molecules (Beta)
- Literature

Comments

H<sub>3</sub>C

- Bioavailability Metric
- Exposure Limit**
- Point Of Departure
- Regulatory Toxicity ...
- Effect Level
- Misc Hazard Informa...
- Screening Level
- Uncertainty Factor

Download as:

### Exposure Limit

Grouping ID	Priority	Type	Subtype	Value	Units	Study Type	Exposure Route	Study Duration	Species	Media	Details	Source
5966	6	tolera...	-	2.00	ul/kg-d...	-	oral	-	-	-	RIVM ...	RIVM
5967	6	tolera...	-	5.00	ul/kg-d...	-	oral	-	-	-	RIVM ...	RIVM
48903	2	MCL-b...	-	1.90e-03	mg/kg...	-	-	-	-	-	RSL d...	RSL
176188	3	water ...	drinkin...	0.7	mg/L	-	oral	chronic	-	drinkin...	EPA D...	ACToR
176190	3	MCL g...	drinkin...	3.00e-03	mg/L	-	oral	-	-	drinkin...	EPA D...	ACToR
176191	3	MCL	drinkin...	3.00e-03	mg/L	-	oral	-	-	drinkin...	EPA D...	ACToR

# The Dashboard in brief

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

## Atrazine

1912-24-9 | DTXSID9020112

© Searched by Approved Name: Found 1 result for 'atrazine'.



### Wikipedia

Atrazine is an herbicide of the triazine class. Atrazine is used to prevent pre- and postemergence broadleaf weeds in crops such as maize (corn) and sugarcane and on turf, such as golf courses and residential lawns. It is one of the most widely used herbicides

- Chemical Properties
- Env. Fate/Transport
- Synonyms
- External Links
- Toxicity Values (Beta)
- Exposure
- Bioassays
- Similar Molecules (Beta)
- Literature



H<sub>3</sub>

### Similar Molecules

Searched with a similarity threshold of 0.82

Download as: TSV Excel

Properties Chemicals

Similarity Value		1	1	1	1	1
LogP: Octanol-Water	Experimental	-	-	1.51	2.61	2.93
	Predicted	-	2.77	1.58	2.76	3.15
Water Solubility	Experimental	-	-	0.00197	0.000130	0.0000374
	Predicted	-	0.0287	0.0108	0.0146	0.000514

# Why should the Dashboard meet NORMAN?

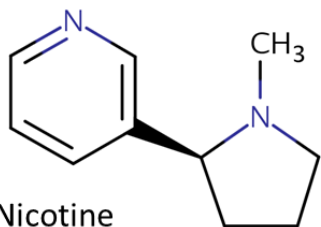
## Common Goals

- Much of the CompTox data is open – as is NORMAN data  
<https://comptox.epa.gov/dashboard/downloads>
- Increase access to data for use in other applications

## Mutual Benefits

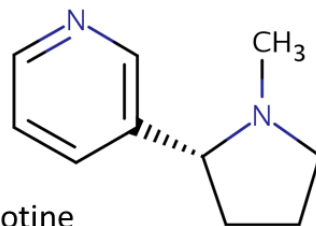
- We have access to data they don't have, within a large European network
- We have additional predictive values & initiatives that are of interest
- They have access to data that we don't have
- They have years of investment/experience in data validation and curation
- They have the ability to provide services currently way beyond our means

# Collaboration on Chemical Curation



Nicotine

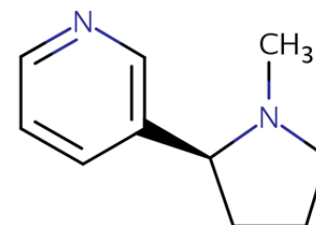
CN1CCC[C@H]1C1=CN=CC=C1  
DTXSID1020930 | SNICXCGAKADSCV  
54-11-5 | **162.1157** | 0.929 | **72**  
Tox: **yes** | Expo: **yes** | Bioassay: **yes**



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**

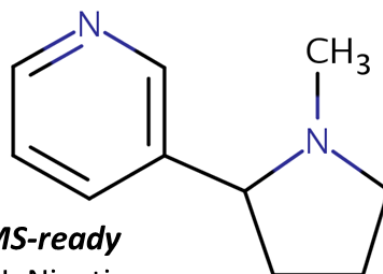
**LEGEND:** Name, SMILES  
DTXSID | InChIKey 1<sup>st</sup> Block  
CAS | **Monoiso. Mass** | logP | **Sources**  
Data on: **Toxicity** | **Exposure** | **Bioassays**



HCl

Nicotine hydrochloride

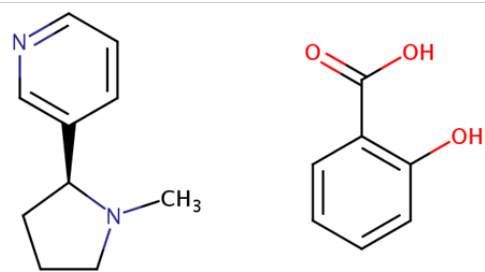
Cl.CN1CCC[C@H]1C1=CN=CC=C1  
DTXSID602093 | HDJBTCAJIMNXEW  
2820-51-1 | **198.0924** | 0.929 | **9**  
Tox: **no** | Expo: **yes** | Bioassay: **yes**



**MS-ready**

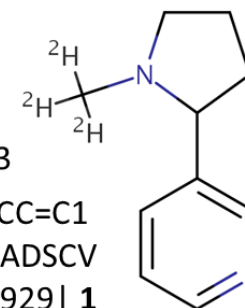
DL-Nicotine

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



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

OC(=O)C1=CC(O)=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**



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**



# Collaboration on Chemical Curation of Lists

Pharmaceutical List with Consumption Data	SwissPharma_TableS2.csv	SwissPharma_TableS2_InChIKeys.txt	Singer <i>et al.</i> 2016. DOI: <a href="https://doi.org/10.1021/acs.est.5b03332">10.1021/acs.est.5b03332</a>
Swiss Insecticides, Fungicides and TPAs	SwissPesticides_TableS1.csv	SwissPesticides_TableS1_InChIKeys.txt	Moschet <i>et al.</i> 2013. DOI: <a href="https://doi.org/10.1021/ac4021598">10.1021/ac4021598</a>
NormaNEWS for retrospective screening of new emerging contaminants	NormaNEWS_V4_26042017.csv	NormaNEWS_V4_InChIKeys.txt	NormaNEWS list provided by Nikiforos Alygizakis, Saer Samanipour and Kevin Thomas
Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006)	Merged_CosmeticProducts_04052017.csv	Merged_CosmeticProducts_04052017_InChIKeys.txt	The scientific committee on cosmetic products and non-food products Intended for consumers - <b>SCCNFP/0389/00 Final</b> and Commission <b>Decision 2006/257/EC</b> amending the Decision 96/335/EC. Provided by Peter von der Ohe, UBA, curated by Reza Aalizadeh, University of Athens
PFAS Highly fluorinated substances list: KEMI	PFAS_Market_Kemi_EPA_1Feb2017.xlsx <b>~2,600 PFAS</b>	Curation in progress: coming soon	Appendix 2 from Swedish Chemicals Agency <b>KEMI Report 7/15</b> . Provided by Stellan Fischer, KEMI
NORMAN Priority List 2015	NORMAN_PriorityList_2016.csv Further curation in progress...	NORMAN_PriorityList_2016_InChIKeys.txt	Priority substances from NORMAN WG-1 (Prioritisation), provided by Valeria Dulio
French Monitoring List	French_List_08052017.csv Further curation in progress...	FrenchList_UniqueInChIKeys_08052017.txt	Provided by Valeria Dulio, curated by Reza Aalizadeh, University of Athens
KEMI Market List	KEMI_MarketList_12052017_MSready.xlsx	KEMI_MarketList_12052017_MSready_InChIKeys.txt	Provided by Stellan Fischer, KEMI including Hazard and Exposure scores, documented <b>here</b> . Curated by Reza Aalizadeh, University of Athens.
TSCA Surfactants	Coming soon...		Provided by Lee Ferguson, sourced from James Little

**24,883 Substances (Expo, Hazard Scores)**



# KEMI PFAS List (Stellan Fischer)

## Norman Network PFAS (KEMI)

Search SFISHFLUORO Chemicals



### List Details

Description: This list of perfluorinated substances originated from Appendix 2 from Swedish Chemicals Agency Report 7/15 (available at <http://www.kemi.se/en/global/rapporter/2015/report-7-15-occurrence-and-use-of-highly-fluorinated-substances-and-alternatives.pdf>) on the occurrence and use of highly fluorinated substances and alternatives (2015). The current KEMI PFAS list includes substances beyond the original report and was provided by Stellan Fischer.

Number of Chemicals: 2257

Sort Options ▼ Select/Deselect All Download as: TSV ▼ Excel ▼ SDF ▼

View Selected



Tetrafluoroethylene  
116-14-3



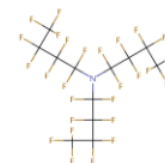
Pentafluoroethane  
354-33-6



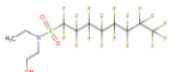
1,1,2,3,3,3-Hexafluoro-1-propene  
116-15-4



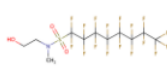
1-Octanesulfonyl fluoride, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8...  
307-35-7



Perfluorotributylamine  
311-89-7



2-(N-Ethylperfluoro-1-octanesulfonamido)ethanol  
1691-99-2



N-Methylperfluorooctanesulfonamidoethanol  
24448-09-7

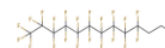


No Chemical Structure Associated with this Substance

Perfluoro compounds, C5-18  
86508-42-1



1,1,2,2-Tetrahydroperfluoro-1-decanol  
678-39-7



1,1,2,2-Tetrahydroperfluoro-1-dodecanol  
865-86-1



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# NormaNEWS

NormaNEWS for retrospective screening of new emerging contaminants	NormaNEWS_V4_26042017.csv	NormaNEWS_V4_InChIKeys.txt	NormaNEWS list provided by Nikiforos Alygizakis, Saer Samanipour and Kevin Thomas
--	---------------------------	----------------------------	---

INPUT	DTXSID	PREFERRED NAME	CASRN	IUPAC NAME	SMILES
DTXSID40881097	<a href="#">DTXSID40881097</a>	C11-LAS	NOCAS_881097	-	CCCCCCC(CCCC)C1=CC=C(C=C1)S(O)(=O)=O
DTXSID30860093	<a href="#">DTXSID30860093</a>	4-(Dodecan-6-yl)benz	23003-92-1	4-(Dodecan-	CCCCCCC(CCCC)C1=CC=C(C=C1)S(O)(=O)=O
DTXSID80881096	<a href="#">DTXSID80881096</a>	C13-LAS	NOCAS_881096	-	CCCCCCCCC(CCC)C1=CC=C(C=C1)S(O)(=O)=O
DTXSID20881095	<a href="#">DTXSID20881095</a>	C14-LAS	NOCAS_881095	-	CCCCCCCCCCC(CCC)C1=CC=C(C=C1)S(O)(=O)=O
DTXSID60881094	<a href="#">DTXSID60881094</a>	SPA-8C	NOCAS_881094	-	CCCC(CCCC(O)=O)C1=CC=C(C=C1)S(O)(=O)=O
DTXSID50865484	<a href="#">DTXSID50865484</a>	10-hydroxycarbazepin	29331-92-8	10-Hydroxy-	NC(=O)N1C2=CC=CC=C2CC(O)C2=CC=CC=C12
DTXSID00881093	<a href="#">DTXSID00881093</a>	Desacetyl diltiazem	42399-40-6	-	[H]C@11(SC2=C(C=CC=C2)N(CCN(C)C)C(=O)C@H

## NormaNEWS: Norman Early Warning System



### List Details

**Description:** The Norman Early Warning System (NormaNEWS) is a pilot network designed to investigate the spatial and temporal distribution of newly identified contaminants of emerging concern in environmental samples through performing retrospective suspect screening on HRMS data acquired using different instrumental platforms and data processing software. The NormaNEWS pilot study was performed through recruiting eight reference laboratories with available archived HRMS data with the goal of exploring the potential of an early warning network to rapidly establish the occurrence of newly-identified contaminants of emerging concern across Europe and beyond, through the use of retrospective suspect screening employing HRMS. The pilot study was referred to as the Norman Early Warning System, abbreviated to NormaNEWS.

**Number of Chemicals:** 131

# NormaNEWS

Dashboard | NORMANEWS

## NORMANEWS

Search NORMANEWS Chemicals



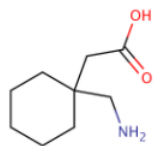
### List Details

**Description:** The Norman Early Warning System (NormaNEWS: <http://www.norman-network.com/?q=node/244>) is a pilot network designed to investigate the spatial and temporal distribution of newly identified contaminants of emerging concern in environmental samples through performing retrospective suspect screening on HRMS data acquired using different instrumental platforms and data processing software. The NormaNEWS pilot study was performed through recruiting eight reference laboratories with available archived HRMS data with the goal of exploring the potential of an early warning network to rapidly establish the occurrence of newly-identified contaminants of emerging concern across Europe and beyond, through the use of retrospective suspect screening employing HRMS. The pilot study was referred to as the Norman Early Warning System, abbreviated to NormaNEWS.

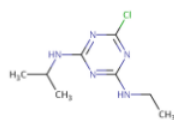
**Number of Chemicals:** 131

Sort Options ▾ Select/Deselect All Download as: TSV ▾ Excel ▾ SDF ▾

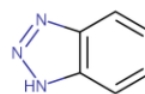
View Selected



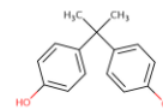
Gabapentin  
60142-96-3



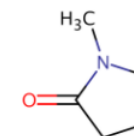
Atrazine  
1912-24-9



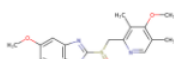
1,2,3-Benzotriazole  
95-14-7



Bisphenol A  
80-05-7



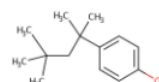
N-Methyl-2-pyrrolidone  
872-50-4



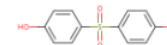
Omeprazole  
73590-58-6



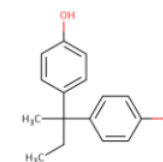
4-Octylphenol  
1806-26-4



4-(1,1,3,3-Tetramethylbutyl)phenol  
140-66-9



4,4'-Sulfonyldiphenol  
80-09-1



Bisphenol B  
77-40-7



# List Functionality in the Dashboard

An overview of all the lists ...

https://comptox.epa.gov/dashboard/chemical\_lists

90%

Search

☆ | 📄 | ✓ | ↓

Search Chemistry Dashboard

## Chemistry Dashboard

### Select List

List Name	Number of Chemicals	List Description
<a href="#">CHEMINV: EPA Chemical Inventory for ToxCast (20170203)</a>	5231	CHEMINV is full list of unique DSSTox substances mapped to historical chemical inventory of physical samples registered by EPA's ToxCast Chemical Contractor (Evotec) since launch of ToxCast program in 2007.
<a href="#">DNT Screening Library</a>	1476	DNTSCREEN is a list of chemicals that is being used in medium- and high-throughput in vitro and zebrafish assays.
<a href="#">EPA Toxcast Screening Library</a>	4736	TOXCAST includes all EPA-provided chemicals for which screening data have been generated in the ToxCast research program since 2007.
<a href="#">Norman Network PFAS (KEMI)</a>	2257	Perfluorinated substances from a Swedish Chemicals Agency Report (provided by Stellan Fischer) on the occurrence and use of highly fluorinated substances.
<a href="#">NORMANews</a>	131	The NORMAN Early Warning System (NormaNEWS) is a collaborative activity run by the NORMAN Network to investigate newly identified contaminants of emerging concern via retrospective screening on HRMS data.
<a href="#">Tox21 Screening Library</a>	8947	TOX21SL is list of unique substances in Tox21 multi-federal agency screening library, contributed by the EPA, National Toxicology Program (NTP), and National Center for Advances in Translational Science (NCATS).

More lists become available with every release

# List Functionality in the Dashboard

Obtaining all chemicals from a given list (downloadable as XLS or SDF)

https://comptox.epa.gov/dashboard/chemical\_lists/toxcast

Chemistry Dashboard | TOXCAST

## EPA Toxcast Screening Library

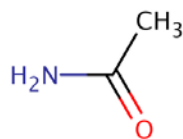
Search TOXCAST Chemicals



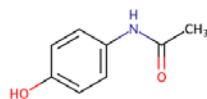
### List Details

Descriptor  
screened in  
limited screen  
volatility, ste  
complete su  
ToxCast ver  
al., Chem. F  
https://www.

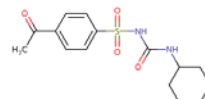
Number of



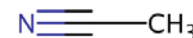
Acetamide  
60-35-5



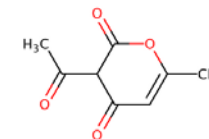
Acetaminophen  
103-90-2



Acetohexamide  
968-81-0



Acetonitrile  
75-05-8

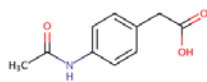


Dehydroacetic acid  
520-45-6

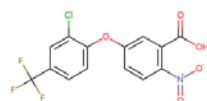


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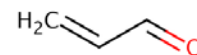
Sort C



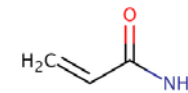
4-Acetylamino-phenylacetic acid  
18699-02-0



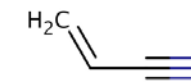
Acifluorfen  
50594-66-6



Acrolein  
107-02-8



Acrylamide  
79-06-1



Acrylonitrile  
107-13-1



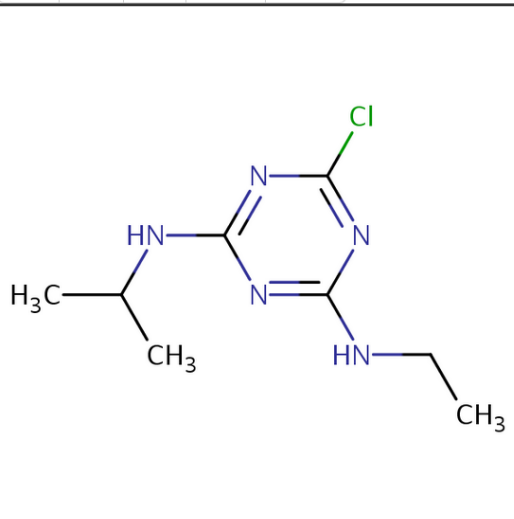
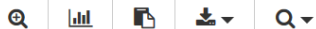
# List Functionality in the Dashboard

## Individual Chemical Level

Atrazine

1912:24:9|DTXSID9020112

© Searched by Approved Name: Found 1 result for 'atrazine'.



Wikipedia

Intrinsic Properties

Structural Identifiers

Related Compounds (Beta)

Presence in Lists

DNT Screening Library

CHEMINV: EPA Chemical Inventory for ToxCast (20170203)

EPA ToxCast Screening Library

Tox21 Screening Library

Record Information



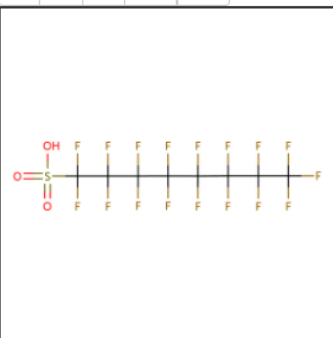
# List Functionality in the Dashboard

Individual Chemical Level ... example from NORMAN lists...

PFOS

1763-23-1 | DTXSID3031864

Searched by Approved Name: Found 1 result for 'PFOS'.



- Wikipedia
- Intrinsic Properties
- Structural Identifiers
- Related Compounds (Beta)
- Presence in Lists
  - [DNT Screening Library](#)
  - [CHEMINV. EPA Chemical Inventory for ToxCast \(20170203\)](#)
  - [EPA ToxCast Screening Library](#)
  - [Tox21 Screening Library](#)
  - [NORMANews](#)
  - [Norman Network PFAS \(KEMI\)](#)
- Record Information

- Chemical Properties
- Env. Fate/Transport
- Synonyms
- Exposure
- Toxicity Values (Beta)
- Bioassays
- External Links
- Similar Molecules (Beta)
- Literature
- Comments

**Summary**

- LogP: Octanol-Water
- Water Solubility
- Density
- Melting Point

Download as:

Property	Average		Median		Range		Unit
	Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
LogP: Octanol-Water	-	4.44 (4)	-	4.44	-	2.32 to 6.28	-
Water Solubility	-	2.41e-03 (4)	-	2.41e-03	-	6.25e-09 to 9.12e-03	mol/L
Density	-	1.84 (1)	-	1.84	-	-	g/cm <sup>3</sup>
Melting Point	-	65.5 (3)	-	65.5	-	51.9 to 73.5	°C

# NORMAN Lists in the Dashboard ...

Coming soon ... (or just released ...)

## Norman Network PFAS (KEMI Report)

### Norman Network PFAS (KEMI Report)

Perfluorinated substances from a Swedish Chemicals Agency Report (provided by Stellan Fisher) on the occurrence and use of highly fluorinated substances.

Wikipedia

Intrinsic Properties

Structural Identifiers

Related Compounds (Beta)

Presence in Lists

DNT Screening Library

CHEMINV. EPA Chemical Inventory for ToxCast (20170203)

EPA ToxCast Screening Library

Tox21 Screening Library

NORMANews

Norman Network PFAS (KEMI)

NORMANews

The NORMAN Early Warning System (NormaNEWS) is a collaborative activity run by the NORMAN Network to investigate newly identified contaminants of emerging concern via retrospective screening on HRMS data.

Record Information

# Future work ... integrating DTXSIDs into NORMAN Lists

Undefined mixtures (UVCBs)

Cleaning up lists to remove errors

Mol_ID	Name	EDITED NAMES FOR INPUT INTO SEARCH	CAS_RN	Merged DTXSIDs	DTXSID Based on Name	Preferred Name
SA8750	By-Product	By-Product	NA	-	-	NO_MATCH
stpQQR1546	C10-DATS C10-Dialkyl tetr	C10-DATS C10-Dialkyl tetralin sulfonate 8	NA	-	-	NO_MATCH
SA2074	C10-LAS	C10-LAS	NA	-	-	NO_MATCH
stpQQR1582	C10LAS C10-linear alkylbe	C10LAS C10-linear alkylbenzyl sulfonate 4	NA	-	-	NO_MATCH
SA14931	C10-phosphonic	C10-phosphonic	NA	-	-	NO_MATCH
StpBB815	C12-15 ALKYL BENZOATE	C12-15 ALKYL BENZOATE	68411-27-8	-	-	NO_MATCH
SA13282	C12-AE5S	C12-AE5S	NA	-	-	NO_MATCH
stpQQR1548	C12-LAS C12-linear alkyl b	C12-LAS C12-linear alkyl benzene sulfonat	NA	-	-	NO_MATCH
stpQQR690	C14-SAS (TENTATIVE) tetr	C14-SAS (TENTATIVE) tetradecane-7-sulfo	NA	-	-	NO_MATCH
stpQQR1557	C16EOx C16EO2 C16-alcc	C16EOx C16EO2 C16-alcohol polyethoxyl	NA	-	-	NO_MATCH
stpQQR1556	C18EOx C18EO2 C18-alcc	C18EOx C18EO2 C18-alcohol polyethoxyl	4439-32-1	-	-	NO_MATCH
SA14932	C4-phosphonic	C4-phosphonic	NA	-	-	NO_MATCH
SA14929	C6-phosphonic	C6-phosphonic	NA	-	-	NO_MATCH
stpQQR1583	C7SPC C7-sulfophenyl car	C7SPC C7-sulfophenyl carboxylates 4-(de	NA	-	-	NO_MATCH
SA14930	C8-phosphonic	C8-phosphonic	NA	-	-	NO_MATCH
stpQQR1547	C8-SPC C8-Sulfophenyl ca	C8-SPC C8-Sulfophenyl carboxylic acid 4-(	NA	-	-	NO_MATCH
stpQQR1576	CA5PE2C 7-{4-[2-(carboxy	CA5PE2C 7-{4-[2-(carboxymethoxy)ethoxy	NA	-	-	NO_MATCH
stpQQR1578	CA6PE2	CA6PE2	NA	-	-	NO_MATCH
stpQQR1577	CA6PE2C	CA6PE2C	NA	-	-	NO_MATCH
stpQQR1575	CA8PE2C	CA8PE2C	NA	-	-	NO_MATCH
SA9863	cacotheline	cacotheline	561-20-6	-	-	NO_MATCH
SAn15715	Caerulomycin A	Caerulomycin A	21802-37-9	-	-	NO_MATCH
SA5151	cafedrine	cafedrine	58166-83-9	-	-	NO_MATCH

(many) more registrations...

# Handling of Undefined Mixtures

<https://comptox.epa.gov/dashboard/dsstoxdb/results?utf8=✓&search=C10-12+chloroalkanes>

## C10-12 chloroalkanes

108171-26-2|DTXSID10872316

**i** Searched by DSSTox\_Substance\_Id: Found 1 result for 'DTXSID10872316':

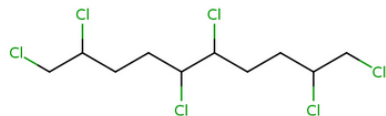
Presence in Lists

Record Information

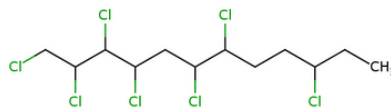
Quality Control Notes

## Related Chemicals

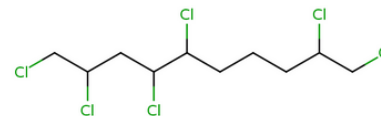
Found 3 chemicals



1,2,5,6,9,10-Hexachlorodecane  
189350-94-5



1,2,3,4,6,7,10-Heptachlorododecane  
1005111-47-6



1,2,4,5,9,10-Hexachlorodecane  
890302-87-1

# Acknowledgements

...after almost 1000 emails, dozens of phone calls, a LOT of extremely valuable input and uncountable hours of late night, after hours work, a HUGE thanks goes to Tony Williams and his team at the Dashboard



Stellan Fischer,  
KEMI



Kevin Thomas (UQ), Saer Samanipour (NIVA), Nikiforos Alygizakis (EI),



Andrew McEachran,  
ORISE Fellow, US EPA

# Questions?

Dashboard:

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

Contact:

[emma.schymanski@eawag.ch](mailto:emma.schymanski@eawag.ch)



**solutions**

EU Grant 603437

# Mixtures (work in progress)

## Mixture identification and curation

- Step 1: Identify all mixture components
- Step 2: Create SMILES, split into components, retain “non-salts”
- Step 3: Create MS-ready identifiers, compare retained components
  - Single structure => all the same, treat as individual
  - Otherwise save as Level 7 for validation ...

