

The EPA Comptox Chemicals Dashboard as a Data Integration Hub for Environmental Chemistry Data

Antony Williams

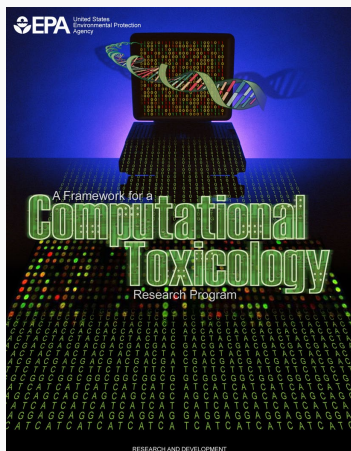
U.S. Environmental Protection Agency, RTP, NC

This work was reviewed by the U.S. EPA and approved for presentation but does not necessarily reflect official Agency policy.

November 5th 2018

National Center for Computational Toxicology

- National Center for Computational Toxicology established in 2005 to integrate:
 - High-throughput and high-content technologies
 - Modern molecular biology
 - Data mining and statistical modeling
 - Computational biology and chemistry
- Currently staffed by ~60 employees as part of EPA's Office of Research and Development
- Home of ToxCast & ExpoCast research efforts
- Key partner in U.S. Tox21 federal consortium
- Multiple cross-division collaborations (e.g. NERL, OPP, OPPT)



The CompTox Portal

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



The CompTox Portal


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



- **A publicly accessible website** delivering access:
 - ~765,000 chemicals with related property data
 - Experimental and predicted physicochemical property 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
 - **DOWNLOADABLE Open Data for reuse and repurposing**

CompTox Chemicals Dashboard


Chemicals


 United States
Environmental Protection
Agency

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
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762 Thousand Chemicals


 **Chemicals** Product/Use Categories Assay/Gene




Bisphenol A
DTXSID7020182




Bisphenol A bis(2-hydroxyethyl ether) diacrylate
DTXSID6066991




Bisphenol A bis(2-hydroxyethyl ether) dimethacrylate
DTXSID1066992




Bisphenol A bis(2-hydroxypropyl) ether
DTXSID8051592




Bisphenol A carbonate polymer
DTXSID6027840




Bisphenol A diglycidyl ether
DTXSID6024624



Bisphenol A glycidyl methacrylate
DTXSID7044841



Bisphenol A propoxylate diglycidyl ether
DTXSID10399098




Bisphenol A propoxylate glycerolate diacrylate
DTXSID40400126

comptox-prod.epa.gov/dashboard

CompTox Chemicals Dashboard


Products and Use Categories



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[Chemicals](#) [Product/Use Categories](#) [Assay/Gene](#)

CPDat PRODUCT category: personal care hair color
hair colors and dyes characterized as permanent

CPDat PRODUCT category: personal care hair color
hair colors and dyes characterized as for professional use

CPDat PRODUCT category: personal care hair color
hair colors and dyes characterized as temporary

CPDat PRODUCT category: personal care hair color
hair coloring products not otherwise categorized

CPDat PRODUCT category: personal care hair color activator
chemical activators for hair coloring products

CPDat PRODUCT category: personal care hair color developer
chemical developers for hair coloring products

CPDat PRODUCT category: personal care hair color toner
chemical toners for hair coloring products

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CompTox Chemicals Dashboard


Assays and Genes



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762 Thousand Chemicals

Chemicals

Product/Use Categories

Assay/Gene

GENE: ESR1
estrogen receptor 1


GENE: ESR2
estrogen receptor 2 (ER beta)

GENE: ESRRB
estrogen-related receptor alpha

GENE: ESRRB
estrogen-related receptor beta

GENE: ESRRG
estrogen-related receptor gamma

and curating data, major updates to the batch searching functionality and access to real time predictions for both physiochemical and toxicity endpoints. A [list of release notes](#) is available for your review. We look forward to your feedback.



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Detailed Chemical Pages

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

► ADME

► EXPOSURE

► BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

► LITERATURE

LINKS

COMMENTS

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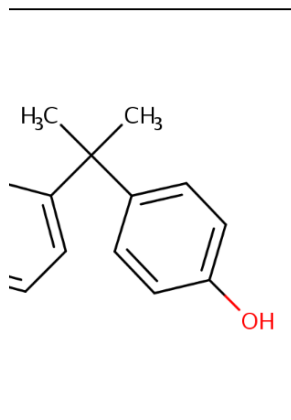
Submit Comment

Search all data

ol A

TXSID7020182

Tox Substance Id.



Wikipedia

Bisphenol A (BPA) is an organic synthetic compound with the chemical formula $(\text{CH}_3)_2\text{C}(\text{C}_6\text{H}_4\text{OH})_2$ belonging to the group of diphenylmethane derivatives and bisphenols, with two hydroxyphenyl groups. It is a colorless solid that is soluble in organic solvents, but poorly soluble in water. It has been in commercial use since 1957.

BPA is a starting material for the synthesis of plastics, primarily

[Read more](#)

Intrinsic Properties

Structural Identifiers

Linked Substances

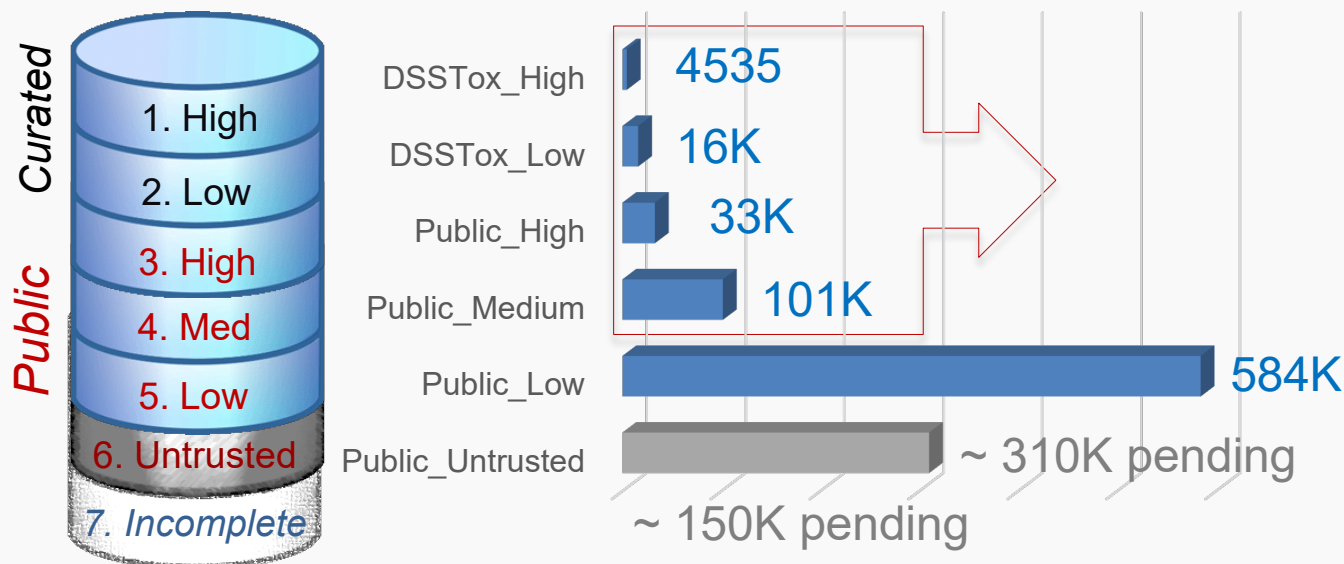
Presence in Lists

Record Information

Quality Control Notes

Almost 20 Years of Data...

Growing with daily curation



QC Levels

DSSTox_High:	Hand curated and validated
DSSTox_Low:	Hand curated and confirmed using multiple public sources
Public_High:	Extracted from EPA SRS and confirmed to have no conflicts in ChemID and PubChem
Public_Medium:	Extracted from ChemID and confirmed to have no conflicts in PubChem
Public_Low:	Extracted from ACToR or PubChem
Public_Untrusted:	Postulated, but found to have conflicts in public sources

Physicochemical and Environmental Fate/Transport Properties

- Solubility
- Melting Point
- Boiling Point
- LogP (Octanol-water partition coefficient)
- Atmospheric Hydroxylation Rate
- LogBCF (Bioconcentration Factor)
- Biodegradation Half-life
- Henry's Law Constant
- Fish Biotransformation Half-life
- LogKOA (Octanol/Air Partition Coefficient)
- LogKOC (Soil Adsorption Coefficient)
- Vapor Pressure

- And more...

Full transparency for predictions

EPA United States Environmental Protection Agency

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Share Search all data

OPERA Models: LogP: Octanol-Water

N-Methyl-2-pyrrolidone
872-50-4 | DTXSID6020856

Save PDF

Model Results

Predicted value: -0.300

Global applicability domain: **Inside**

Local applicability domain index: 0.88

Confidence level: 0.81

Model Performance

Weighted KNN model

QMRP

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Nearest Neighbors from the Training Set

CN1CCCC1=O
N-Methyl-2-pyrrolidone
Measured: -0.380
Predicted: -0.300

O=C1CCCCN1
Prolinal
Measured: -0.320
Predicted: -0.226

CCN1CCCC1=O
1-Ethyl-2-pyrrolidinone
Measured: -0.0400
Predicted: -0.211

C=CN1CCCC1=O
N-Vinyl-2-pyrrolidone
Measured: 0.37
Predicted: 2.65e-01


Transparency: QMRF Report

QMRF_NCCT_MP_08212016 - Adobe Acrobat Pro

File Edit View Window Help

Create [Icons] Customize [Icon]

1 / 10 [Icons] 143% [Icons] Tools Fill & Sign Comment

	<i>QMRF identifier (JRC Inventory): To be entered by JRC</i>
	<i>QMRF Title: MP: Melting point prediction from the NCCT Models Suite.</i>
	<i>Printing Date: May 4, 2016</i>

1. QSAR identifier

1.1. QSAR identifier (title):
MP: Melting point prediction
from the NCCT_Models Suite.

1.2. Other related models:
No related models

1.3. Software coding the model:
NCCT_models V1.02
Suite of QSAR models to predict physicochemical properties and environmental fate of organic
chemicals

- Our approach to modeling:
 - Obtain **high quality** training sets
 - Apply appropriate modeling approaches
 - **Validate** performance of models
 - Define the applicability domain and model limitations
 - Use models to predict properties across our full datasets
 - Release as **Open Data and Open Models**

EPI Suite Data - ISIS/Base & SDF

The downloaded files are provided in "zip" format ... the downloaded file must be "un-zipped" with common utility programs such as [WinZip](#).

... *Updated September 15, 2010*

Basic Instructions:

- (1) Download the zip file
- (2) Un-Zip the file

NOTE ... zipped files extract to Folders containing the individual data files ... Folders named EPI_ISIS_Data and EPI_SDF_Data

Substructure Searching Files:

ISISTM/Base & SD Files of the EPI Suite Program Experimental Data Files are now available ... The ISISTM/Base files require the commercial program for use ... The SD Files can be imported into other commercial chemical structure programs (such as ChemFinder).

... [Click here to download EPI_ISIS_Data.zip](#) ... (about 11 MB)

... [Click here to download EPI_SDF_Data.zip](#) ... (about 10 MB)

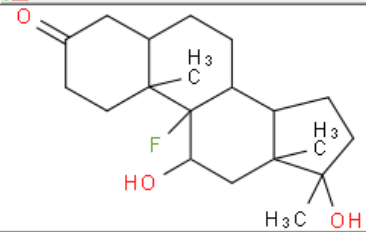
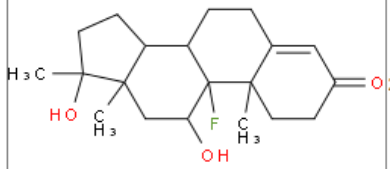
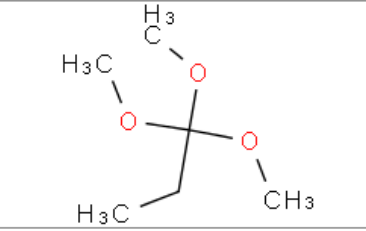
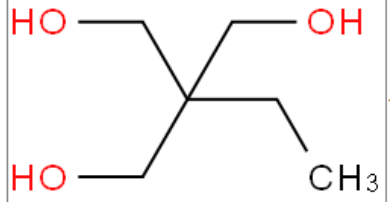
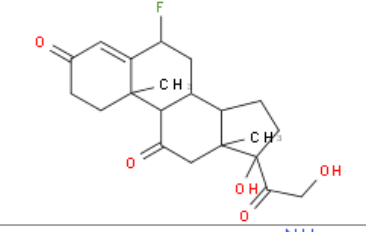
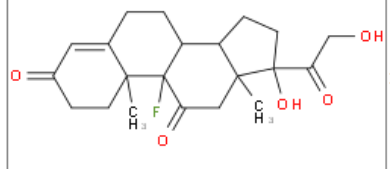
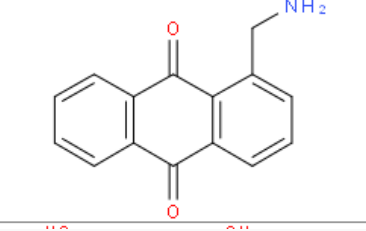
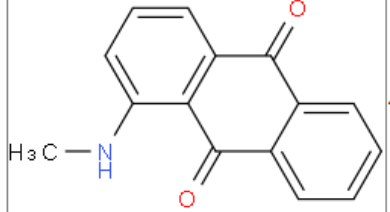
NOTE ... EPI Suite Data Files (some in Excel, Text, Word format) available at:

<http://esc.syrres.com/interkow/EpiSuiteData.htm>

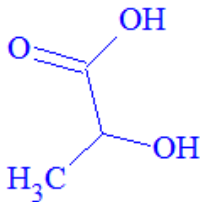
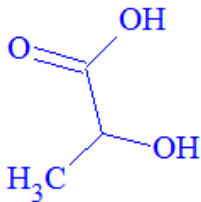
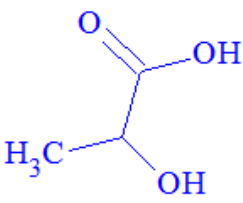
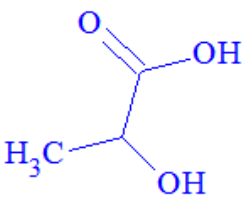
We Curated These Public Data to Build Prediction Models

Public data should be curated prior to modeling



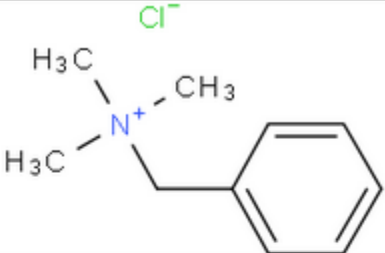
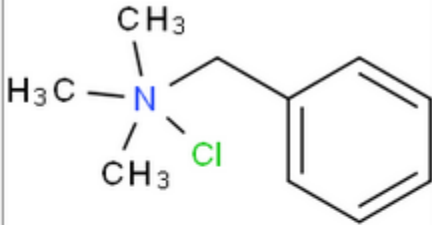
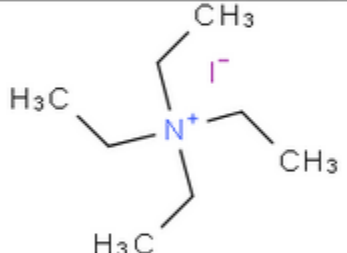
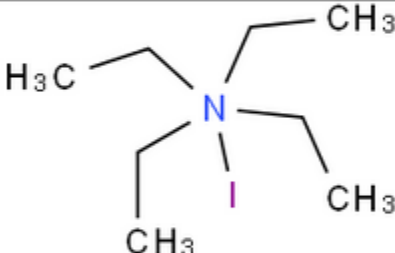
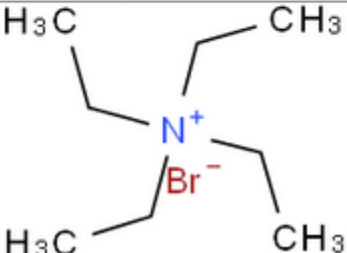

Different Compounds

Mol Block	S CAS	S NAME	Smiles
	000076-43-7	FLUOXYMESTERONE	
	000077-99-6	1,1,1-TRIS(HYDROXYMETHYL)PROPANE	
	000079-60-7	CORTISONE-9A-FLUORO	
	000082-38-2	DISPERSE RED 9	

Duplicate Structures

Structure	Formula <	FW <	CAS <	NAME <	MP <	EstMP <	ErrorMP <
	C ₃ H ₆ O ₃	90.0779	000050-21-5	LACTIC ACID	1.6800000000000000e+001	2.2660000000000000e+001	5.8600000000000000e+000
	C ₃ H ₆ O ₃	90.0779	000079-33-4	L-LACTIC ACID	5.3000000000000000e+001	2.2660000000000000e+001	-3.0340000000000000e+001
	C ₃ H ₆ O ₃	90.0779	000598-82-3	A-HYDROXYPROPIONIC ACID	1.8000000000000000e+001	2.2660000000000000e+001	4.6600000000000000e+000
	C ₃ H ₆ O ₃	90.0779	010326-41-7	D-LACTIC ACID	5.2800000000000000e+001	2.2660000000000000e+001	-3.0140000000000000e+001

Covalent Halogens

 Mol Block	S CAS	S NAME	 Smiles
 <p>Chemical structure of Benzyltrimethylammonium chloride (Mol Block): A central nitrogen atom (N⁺) is bonded to three methyl groups (H₃C) and a benzyl group (CH₂-C₆H₅). A chloride ion (Cl⁻) is shown as a separate species.</p>	000056-93-9	BENZYL TRIMETHYL AMMONIUM CHLORIDE	 <p>Chemical structure of Benzyltrimethylammonium chloride (Smiles): A central nitrogen atom (N) is bonded to three methyl groups (CH₃) and a benzyl group (CH₂-C₆H₅). A chloride ion (Cl) is shown as a separate species.</p>
 <p>Chemical structure of Tetraethylammonium iodide (Mol Block): A central nitrogen atom (N⁺) is bonded to four ethyl groups (CH₃-CH₂). An iodide ion (I⁻) is shown as a separate species.</p>	000068-05-3	TETRAETHYL AMMONIUM IODIDE	 <p>Chemical structure of Tetraethylammonium iodide (Smiles): A central nitrogen atom (N) is bonded to four ethyl groups (CH₃-CH₂). An iodide ion (I) is shown as a separate species.</p>
 <p>Chemical structure of Tetraethylammonium bromide (Mol Block): A central nitrogen atom (N⁺) is bonded to four ethyl groups (CH₃-CH₂). A bromide ion (Br⁻) is shown as a separate species.</p>	000071-91-0	TETRAETHYL AMMONIUM BROMIDE	 <p>Chemical structure of Tetraethylammonium bromide (Smiles): A central nitrogen atom (N) is bonded to four ethyl groups (CH₃-CH₂). A bromide ion (Br) is shown as a separate species.</p>

Curation to QSAR Ready Files

Property	Initial file	Curated Data	Curated QSAR ready
AOP	818	818	745
BCF	685	618	608
BioHC	175	151	150
Biowin	1265	1196	1171
BP	5890	5591	5436
HL	1829	1758	1711
KM	631	548	541
KOA	308	277	270
LogP	15809	14544	14041
MP	10051	9120	8656
PC	788	750	735
VP	3037	2840	2716
WF	5764	5076	4836
WS	2348	2046	2010

LogP dataset: 15,809 structures

- CAS Checksum: 12163 valid, 3646 invalid (**>23%**)
- Invalid names: 555
- Invalid SMILES 133
- Valence errors: 322 Molfile, 3782 SMILES (**>24%**)
- Duplicates check:
 - 31 DUPLICATE MOLFILES
 - 626 DUPLICATE SMILES
 - 531 DUPLICATE NAMES
- SMILES vs. Molfiles (structure check)
 - 1279 differ in stereochemistry (**~8%**)
 - 362 “Covalent Halogens”
 - 191 differ as tautomers
 - 436 are different compounds (**~3%**)

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

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

 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

OPERA Models: <https://github.com/kmansouri/OPERA>

Other Data: Human and Ecological Chemical Hazard Data

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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

Data Type











Point of Departure ▼


Download ▼

HumanEco

Columns ▼10 ▼

Search query

More ▼	Priority ▼	Toxval type ▼	Subtype ▼	Risk assessment class ▼	Value ^	Units ▼	Study type ▼	Exposure route ▼	Species ▼	Subsource ▼	Source ▼
	5	BMDL-10	-	chronic	0.609	mg/kg-day	human	-	mouse	EFSA CEF	EFSA
	5	NOEL	Systemic	repeat dose	3.75	mg/kg-day	repeat dose toxicity : oral	oral	rat	-	ECHA
	6	NOAEL	-	reproductive	3.75	mg/kg-day	reproductive	oral	rat	-	HPVIS
	5	NOEL	Systemic	repeat dose	3.75	mg/kg-day	repeat dose toxicity : oral	oral	rat	-	ECHA
	5	NOEL	Systemic	repeat dose	4.5	mg/kg-day	repeat dose toxicity : oral	oral	mouse	-	ECHA
	5	NOEL	Systemic	repeat dose	4.5	mg/kg-day	repeat dose toxicity : oral	oral	mouse	-	ECHA
	7	LEL	-	subchronic	5	mg/kg-day	subchronic	oral	rat	unpublished_submission	ToxRefDB
	7	nel	-	chronic	5	mg/kg-day	reproductive multigeneration	oral	rat	open_lit	ToxRefDB
	5	NOAEL	-	chronic	5	mg/kg-day	human	-	mouse	EFSA AFC	EFSA
	7	nel	-	subchronic	5	mg/kg-day	subchronic	oral	rat	unpublished_submission	ToxRefDB



- ToxVal Database contains following data:
 - 30,050 chemicals
 - 772,721 toxicity values
 - 29 sources of data
 - 21,507 sub-sources
 - 4585 journals cited
 - 69,833 literature citations
- If only the data were easy to extract...

- Chemicals in commerce, of interest to the EPA, are not all easily represented by structures
- Different chemical substances supported
 - “UVCB chemicals” - Unknown or Variable Composition, Complex Reaction Products and Biological Materials
 - Homologous series as Markush Structures

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

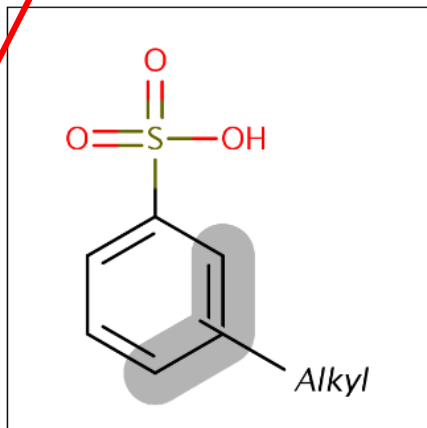
↳ Ethene, tetrafluoro-, oxidized, polymd., reduced, decarboxylated, C6 fraction
274917-96-3 | DTXSID00108075

↳ 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

(C10-C16) Alkylbenzenesulfonic acid

68584-22-5 | DTXSID2028723

Searched by DSS Tox Substance ID.



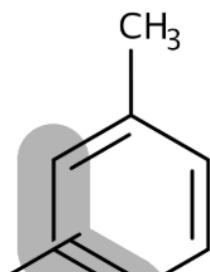
Intrinsic Properties
Presence in Lists
Federal
Safer Choice Chemical List TOX21SL: Tox21 Screening Library TSCA Workplan Step 2 Chemicals
EPAHFR - EPA Chemicals associated with hydraulic fracturing
US State
None.
International
OLEM RapidTox Chemicals REACH Dossier Chemicals
Other
Surfactant List Screened in Swiss Wastewater (2014) EDSP Universe TSCAACTIVE
EPA Chemicals associated with hydraulic fracturing

Markush Structures

Xylenes

1330-20-7 | DTXSID2021446

Searched by DSSTox Substance Id.



Wikipedia

Xylene (from Greek ξύλο, *xylō*, "wood"), **xylo**l or **dimethylbenzene** is any one of three isomers of dimethylbenzene, or a combination thereof. With the formula $(\text{CH}_3)_2\text{C}_6\text{H}_4$, each of the three compounds has a central benzene ring with two methyl groups attached at substituents. They are all colorless, flammable liquids, some of which are of great industrial value. The mixture is referred to as both xylene and, more precisely, xylenes

[Read more](#)

Intrinsic Properties

Presence in Lists

Record Information

DETAILS

RELATED SUBSTANCES

PROPERTIES

COMMENTS

8 chemicals

Download / Send

Show info:

DTXSID

CASRN

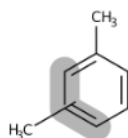
Select all

Sort by: Relationship

Filter by: Name or CASRN

Hide

Searched Chemical



Xylenes

DTXSID: DTXSID2021446
CASRN: 1330-20-7

Predecessor: Component

4 related chemical
structures with this
substance

Xylenes; defined mixture 1
DTXSID: DTXSID0021421
CASRN: NOCAS_21421

Predecessor: Component

4 related chemical
structures with this
substance

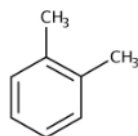
Xylenes; defined mixture 2
DTXSID: DTXSID7021447
CASRN: NOCAS_21447

Predecessor: Component

5 related chemical
structures with this
substance

Total Petroleum Hydrocarbons (TPH)
DTXSID: DTXSID30801529
CASRN: NOCAS_801529

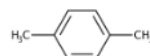
Markush Child



o-Xylene

DTXSID: DTXSID3021807
CASRN: 95-47-6

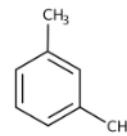
Markush Child



p-Xylene

DTXSID: DTXSID2021888
CASRN: 106-42-3

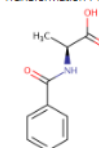
Markush Child



m-Xylene

DTXSID: DTXSID6026298
CASRN: 106-38-3

Transformation Product



N-Benzoylalanine

DTXSID: DTXSID40176394
CASRN: 2198-84-3

Environmental Chemistry:

More about Names and CASRNs

- For EPA most chemicals are reported as text – chemical names and CAS Numbers

Attachment D (Method 3)

SIM quantitation ions and qualifiers for internal standards, references method analysis, and surrogates

<u>Name of Compound</u>	<u>CAS No.</u>	<u>Quantitation Ion</u>	<u>Qualifier Ions</u>
Phenol-d6 (SS)	13187-88-3	99	71, 42
Phenol	108-95-2	94	66
1,4-Dichlorobenzene	106-46-0	146	111, 75, 50
Acetophenone	98-86-2	105	77, 51, 120
Acenaphthene-d10 (IS)	15067-26-2	162	160, 80
p-Cresol	106-44-5	107	108, 77
Isophorone	78-59-1	82	138, 54
Camphor	76-22-2	95	81, 108, 152
Isoborneol	124-76-5	95	110, 121, 136
Menthol	89, 78, 1	71	81, 123, 138
Naphthalene	91-20-3	128	102, 51
Methyl salicilate	119-36-8	120	92, 152, 65

Chemicals in product SDS sheets are commonly UVCBs

Methylparaben

99-76-3 | DTXSID4022529

Searched by Synonym from Valid Source.

 Download ▼

Columns ▼

10 ▼

Product or Use Categorization

[personal care: eye liner](#)

[personal care: body wash](#)

[personal care: sunscreen](#)

[personal care: hair conditioning treatment](#)

[personal care: lip color](#)

182 chemicals in Personal Care: Eye Liner Category

Searched by Product & Use Categories

Results for CPDat Product Category: Personal Care: Eye Liner

182 chemicals

Download / Send

Sort by: DTXSID



Show info:

DTXSID

CASRN

TOXCAST



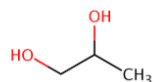
Select all



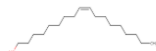
Filter by:

Name or CASRN

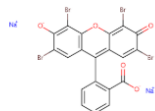
Hide



1,2-Propylene glycol
DTXSID: DTXSID0021206
CASRN: 57-55-6
TOXCAST: 11/539



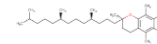
cis-Oleyl alcohol
DTXSID: DTXSID0022010
CASRN: 143-28-2
TOXCAST: 0



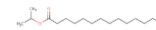
Eosin
DTXSID: DTXSID0025234
CASRN: 17372-87-1
TOXCAST: 45/302

1 related chemical
structure with this
substance

Polyvinylpyrrolidone
DTXSID: DTXSID0025941
CASRN: 9003-39-8
TOXCAST: 0



alpha-Vitamin E
DTXSID: DTXSID0026339
CASRN: 59-02-9
TOXCAST: 0



Isopropyl tetradecanoate
DTXSID: DTXSID0026838
CASRN: 110-27-0
TOXCAST: 1/299

0 related chemical
structures with this
substance

Paraffin waxes and Hydrocarbon waxes...
DTXSID: DTXSID0028115
CASRN: 63231-60-7
TOXCAST: 0

1 related chemical
structure with this
substance

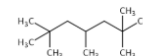
Alcohols, C16-18
DTXSID: DTXSID0028323
CASRN: 67762-27-0
TOXCAST: 1/163

0 related chemical
structures with this
substance

Fats and Glyceric oils, vegetable, hyd...
DTXSID: DTXSID0028454
CASRN: 68334-28-1
TOXCAST: 0



Iron(III) oxide
DTXSID: DTXSID0029632
CASRN: 1309-37-1
TOXCAST: 0



2,2,4,6,6-Pentamethylheptane
DTXSID: DTXSID0042034
CASRN: 13475-82-6
TOXCAST: 0



Squalane
DTXSID: DTXSID0046513
CASRN: 111-01-3
TOXCAST: 2/109

CASRNs can be problematic...

<u>Name of Compound</u>	<u>CAS No.</u>
Phenol-d6 (SS)	13187-88-3
Phenol	108-95-2
1,4-Dichlorobenzene	106-46-0
Acetophenone	98-86-2
Acenaphthene-d10 (IS)	15067-26-2
p-Cresol	106-44-5
Isophorone	78-59-1
Camphor	76-22-2
Isoborneol	124-76-5
Menthol	89, 78, 1
Naphthalene	91-20-3
Methyl salicilate	119-36-8

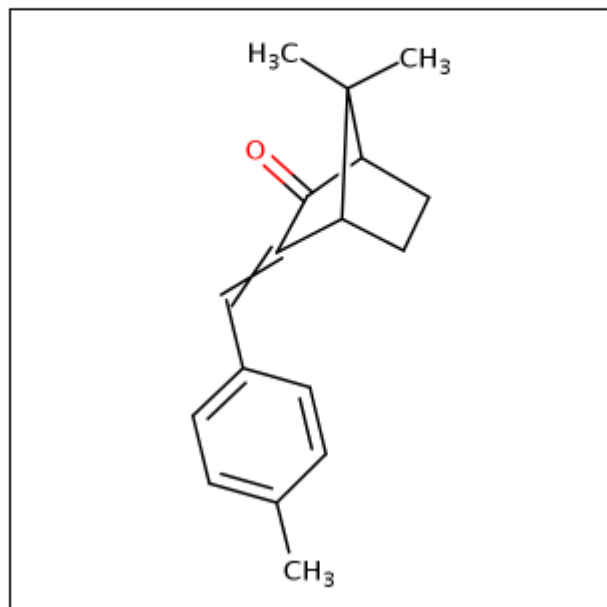
Active vs Deleted CASRN

Also “Alternates”

Enzacamene

36861-47-9 | DTXSID8047896

Searched by Approved Name.



Synonym	Quality
Enzacamene	Valid
7,7-Dimethyl-3-[(4-methylphenyl)methylidene]bicyclo[2.2.1]heptan-2-one	Valid
Bicyclo[2.2.1]heptan-2-one, 7,7-dimethyl-3-[(4-methylphenyl)methylene]-	Valid
36861-47-9 Active CA 8-RN	Valid
Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-3-[(4-methylphenyl)methylene]-	Valid
EINECS 253-242-8	Other
Eusolex 6300	Other
Uvinul MBC 95	Other
Parsol 5000	Other

UNII-813XWY40L9	Other
4-Methylbenzylidenecamphor	Other
p-Methylbenzylidenecamphor	Other
38102-62-4 Deleted CA 8-RN	Deleted
84055-65-2 Deleted CA 8-RN	Deleted

Tricky mapping by CASRN

This one has **316** Deleted CASRN

CAS Registry Number: 25068-38-6

(C₁₅ H₁₆ O₂ · C₃ H₅ Cl O)_x

Phenol, 4,4'-(1-methylethylidene)bis-, polymer with 2-(chloromethyl)oxirane

Polymer

Polymer Class Terms: Epoxy resin

Alternate CAS Registry Numbers: 26402-79-9

Deleted CAS Registry Numbers: 1336-88-5, 1337-15-1, 8000-31-5, 9015-99-0, 9049-54-1, 9050-21-9, 9081-91-8, 9083-76-5, 9084-94-0, 9086-62-8, 9087-26-7, 9087-76-7, 11097-80-6, 11098-13-8, 11098-40-1, 11100-23-5, 11108-41-1, 11120-31-3, 11121-19-0, 11126-36-6, 20232-24-0, 35038-60-9, 36344-96-4, 36347-13-4, 36347-14-5, 37184-50-2, 37184-52-4, 37208-29-0, 37217-92-8, 37230-74-3, 37243-66-6, 37243-67-7, 37251-33-5, 37265-21-7, 37270-82-9, 37291-75-1, 37293-07-5, 37294-18-1, 37305-82-1, 37307-45-2, 37317-45-6, 37325-21-6, 37338-63-9, 37342-17-9, 37345-34-9, 37348-56-4, 37348-57-5, 37357-73-6, 37360-93-3, 39277-59-3, 39288-99-8, 39296-08-7, 39296-09-8, 39296-11-2, 39296-15-6, 39315-77-0, 39349-91-2, 39354-86-4, 39362-25-9, 39362-45-3, 39373-81-4, 39378-29-5, 39378-55-7, 39389-49-6, 39405-18-0, 39412-57-2, 39419-66-4, 39453-22-0, 39454-54-1, 39454-69-8, 39470-62-7, 42612-34-0, 42618-03-1, 50642-36-9, 50642-55-2, 50642-78-9, 51158-20-4, 51273-81-5, 51329-73-8, 51393-99-8, 51394-03-7, 51553-00-5, 52011-87-7, 52038-45-6, 52051-70-4, 52051-82-8, 52052-16-1, 52232-05-0, 52232-75-4, 52276-55-8, 52365-33-0, 52519-66-1, 52519-67-2, 52627-94-8, 52907-38-7, 53027-88-6, 53127-14-3, 53200-30-9, 53238-86-1, 53238-87-2, 53239-67-1, 53239-68-2, 53570-97-1, 53570-98-2, 53681-78-0, 53858-93-8, 54018-73-4, 54352-05-5, 55464-96-5, 55584-55-9, 55585-07-4, 55818-73-0, 56258-35-6, 56449-43-5, 56509-48-9, 57107-66-1, 57284-90-9, 57534-21-1, 57693-04-6, 58052-05-4, 58128-38-4, 58392-89-5, 58392-92-0, 58516-14-6, 58572-71-7, 59029-19-5, 59459-14-2, 59473-30-2, 59948-36-6, 60202-19-9, 60267-31-4, 60382-89-0, 60606-56-6, 60800-54-6, 60831-77-8, 60894-16-8, 61036-82-6, 61287-42-1, 61356-27-2, 61711-38-4, 61763-30-2, 61991-18-2, 62169-28-2, 62169-29-3, 62601-75-6, 62601-76-7, 62887-23-4, 63055-40-3, 63172-55-4, 63799-24-6, 63993-57-7, 63993-58-8, 64086-14-2, 64086-16-4, 64176-52-9, 64176-61-0, 64176-66-5, 64177-03-3, 65233-49-0, 65931-38-6, 65931-39-7, 66995-96-8, 67185-62-0, 68821-97-6, 69899-40-7, 70179-83-8, 70213-44-4, 70726-45-3, 71965-91-8, 72514-40-0, 73413-19-1, 74504-20-4, 74564-76-4, 75831-44-6, 78564-77-9, 79585-43-6, 80702-61-0, 81458-12-0, 81843-57-4, 81843-58-5, 81855-87-0, 82197-12-4, 82197-46-4, 83202-85-1, 84286-97-5, 84683-04-5, 84931-29-3, 85537-69-5, 86090-60-0, 88385-37-9, 88528-19-2, 88651-18-7, 89750-00-5, 91727-28-5, 91727-29-6, 92481-37-3, 95327-25-6, 96420-31-4, 96510-68-8, 97568-16-6, 97709-01-8, 99400-50-7, 101027-12-7, 102256-87-1, 103599-13-9, 103599-14-0, 104364-97-8, 104491-99-8, 105521-57-1, 106207-08-3, 106856-89-7, 107991-47-9, 108556-05-4, 108728-21-8, 110158-22-0, 111367-08-9, 111517-59-0, 114013-37-5, 115902-32-4, 117216-90-7, 117313-45-8, 117786-92-2, 118340-04-8, 120146-74-9, 120797-43-5, 121181-85-9, 121273-37-8, 121547-73-7, 123939-44-6, 125147-87-7, 127176-80-1, 127176-81-2, 128281-71-0, 132822-20-9, 132893-73-3, 135976-90-8, 137545-29-0, 138157-20-7, 138361-18-9, 139554-29-3, 142540-11-2, 144046-24-2, 144046-25-3, 144855-66-3, 149013-58-1, 150825-32-4, 157321-42-1, 157481-46-4, 158725-45-2, 160674-45-3, 161937-12-8, 162031-55-2, 167972-06-7, 168042-08-8, 179607-24-0, 183581-68-2, 183890-12-2, 187619-11-0, 188448-56-8, 189282-49-3, 191606-83-4, 220090-06-2, 222835-65-6, 222835-66-7, 222835-68-9, 222835-69-0, 222835-70-3, 222835-72-5, 222835-74-7, 222835-77-0, 309945-96-8, 339530-81-3, 353239-57-3, 367523-08-8, 383889-26-7, 383889-27-8, 395069-05-3, 470462-49-8, 681001-41-2, 848887-61-6, 913745-83-2, 917483-69-3, 922728-11-8, 934588-09-7, 945610-97-9, 950907-45-6, 1033821-54-3, 1034342-45-4, 1068160-75-7, 1082736-74-0, 1096473-97-0, 1114797-08-8, 1189565-70-5, 1190235-62-1, 1190729-68-0, 1192045-32-1, 1195324-26-5, 1196030-95-1, 1198291-96-1, 1199811-18-1, 1203835-26-0, 1206700-05-1, 1228639-00-6, 1245563-83-0, 1271727-39-9, 1300093-58-6, 1300102-07-1, 1305321-17-8, 1338071-08-1, 1446691-72-0, 1450839-98-1, 1620807-39-7, 1641551-32-7, 1807886-28-7, 1815624-46-4, 1815624-47-5

In Vitro Bioassay Screening

ToxCast and Tox21

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

TOXCAST: SUMMARY

PUBCHEM

TOXCAST: DATA

TOXCAST: MODELS

SIMILAR COMPOUNDS

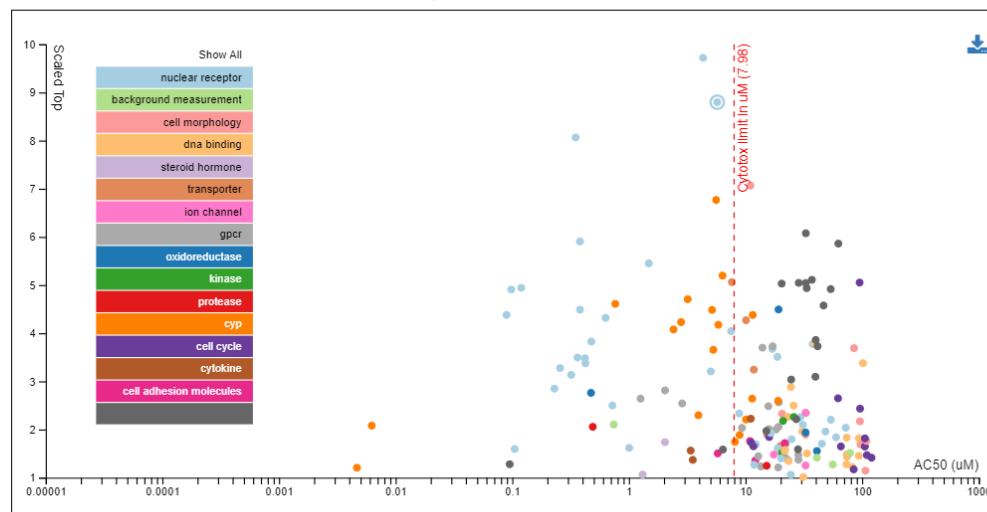
GENRA (BETA)

RELATED SUBSTANCES

Chemical Activity Summary i

TOXCAST DATA


ASSAY DETAILS



AC50 (uM): 5.73
Scaled top: 8.80
Assay Endpoint Name: OT_ER_ERaEra_0480
Assay Description: 742
Gene Symbol: ESR1
Organism: human
Tissue: kidney
Assay Format Type: cell-based
Biological Process Target: protein stabilization
Detection Technology: Protein-fragment Complementation
Analysis Direction: positive
Intended Target Family: nuclear receptor
Description: Data from the assay component OT_ER_ERaEra_0480 was analyzed into 1 assay endpoint. This assay endpoint, OT_ER_ERaEra_0480, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of binding reporter, measures of receptor for gain-of-signal activity can be used to understand the binding at the pathway-level as they relate to the gene ESR1. Furthermore, this assay endpoint can be referred to as a primary readout, because the performed assay has only produced 1 assay endpoint. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the 'nuclear receptor' intended target family, where the subfamily is 'steroidal'.

In Vitro Bioassay Screening

ToxCast and Tox21

United States
Environmental Protection
Agency

HomeAdvanced SearchBatch SearchListsPredictionsDownloads

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Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

QC Data ID	Grade	Description
Tox21_202992	Pass	Purity>90% and MW confirmed
Tox21_400088	Pass	Purity>90% and MW confirmed

Assay Selection 1 SelectedA Single Assay Can Have Multiple ChartsNumber of Charts: 6

☒ Active☐ Inactive☐ All

Filter

Filter assays

Assay Set: ER (1 of 18 Selected)

☒ ACEA_T47D_80hr_Positive

☐ ATG_ERE_CIS_up

☐ ATG_ERa_TRANS_up

☐ NVS_NR_DER

☐ NVS_NR_hER

☐ NVS_NR_mERa

☐ OT_ERaERa_0480

☐ OT_ERaERa_1440

☐ OT_ERaERb_0480

☐ OT_ERaERb_1440

☐ OT_ERaERb_0480

☐ OT_ERaERb_1440

Submit CommentSave ChartSave Data

ACEA_T47D_80hr_Positive
HITCALL: ACTIVE
Bisphenol A (80-05-7)
DTXSID7020182
TX009158

Percentage Activity

Log Concentration (uM)

AC50 (0.42)

Cmax (1.96)

Cmax (116.9)

Cut Off

Constant ModelGain-Loss ModelHill Model

Exploring ToxCast Data: Downloadable Data

The results after processing through the Pipeline are available on the [ToxCast Dashboard](#), and for most users EPA recommends accessing the data there.

- [ToxCast Chemicals](#)
- [ToxCast Assays](#)

ToxCast Data and Information

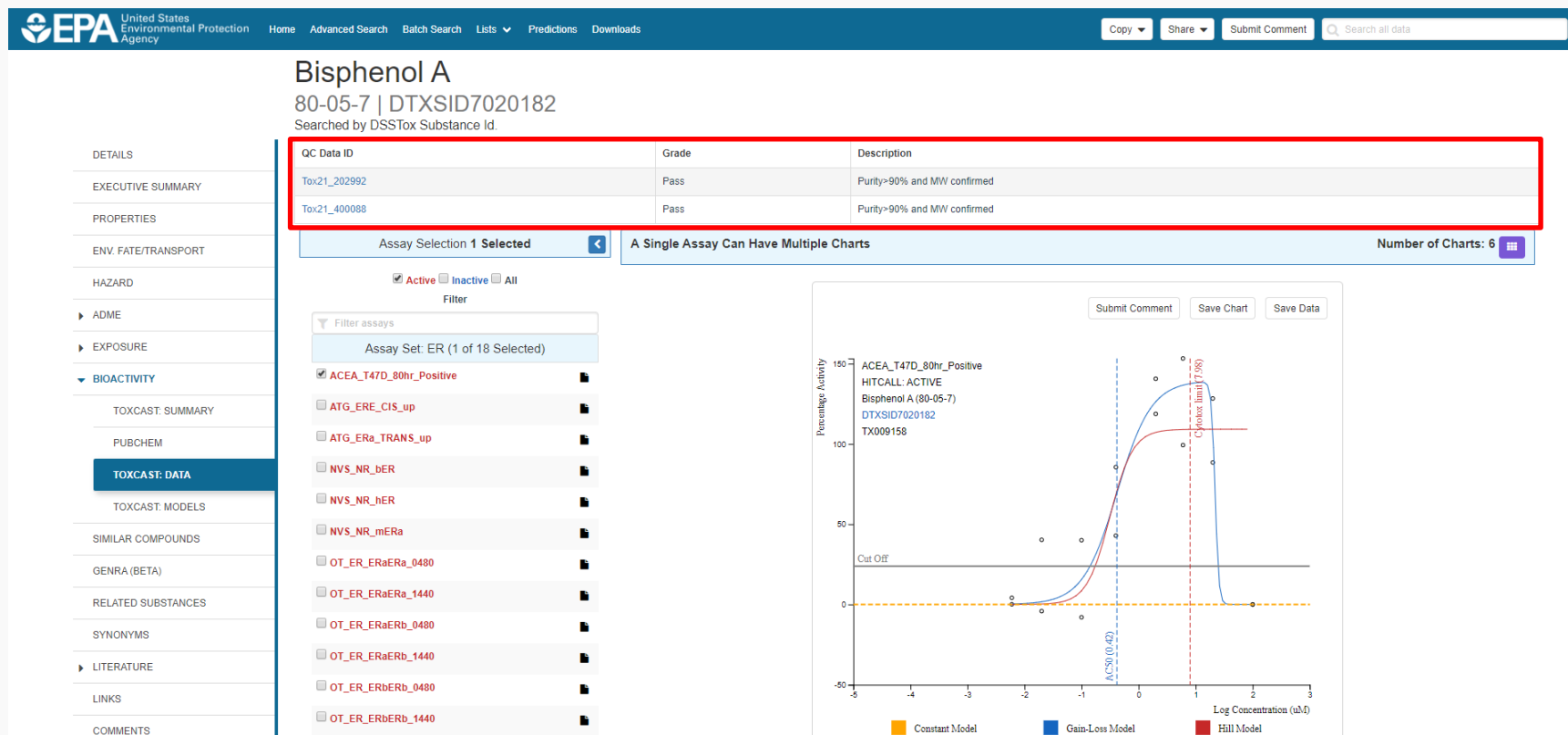
- **ToxCast & Tox21 Summary Files.** Data for a single chemical endpoint pair for thousands of chemicals and assay endpoints for 20 variables such as the activity or hit call, activity concentrations, whether the chemical was tested in a specific assay, etc.
 - [Download ToxCast Summary Information](#)
 - [Download ReadMe](#)
- **ToxCast & Tox21 Data Spreadsheet.** A spreadsheet of EPA's analysis of the chemicals screened through ToxCast and the Tox21 collaboration which includes EPA's activity calls from the screening of over 1,800 chemicals.
 - [Download Data](#)
 - [Download ReadMe](#)
- **ToxCast Data Pipeline R Package.** The R computer programming package used to process and model all EPA ToxCast and Tox21 chemical screening data. The files include the R programming package as well as documents that provide overviews of the data analysis pipeline used and the R package. Users will need experience with R to use these files.
 - [Download Package](#)
 - [TCPL Overview](#)

Resources

- [Toxicity Forecaster \(ToxCast\) Fact Sheet](#)
- [ToxCast Publications](#)
- [ToxCast Citation](#)
- [About ToxCast](#)

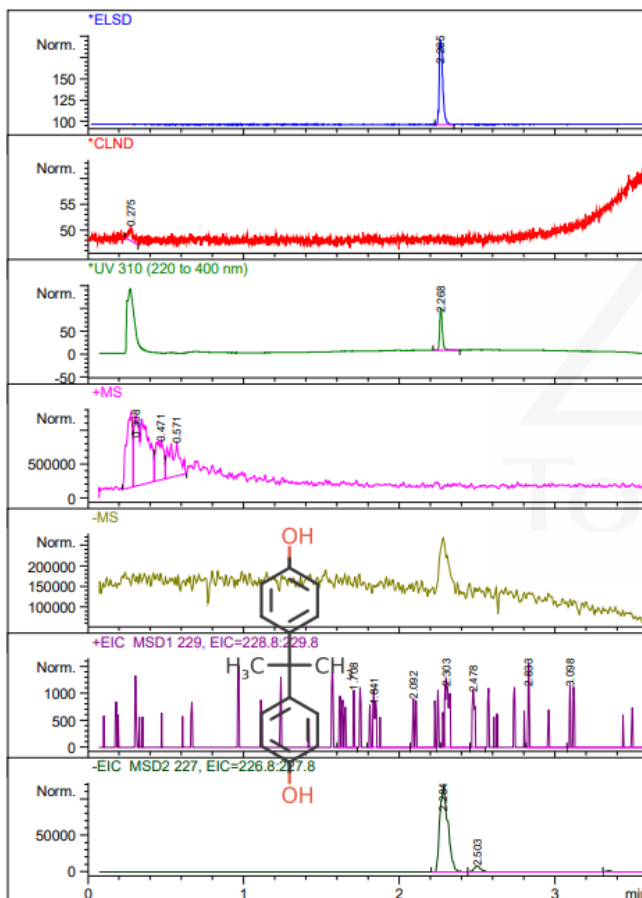
ToxCast/Tox21 Data

Analytical QC of the chemicals



Access to Analytical QC Data

ID Tox21_202992 Plate Batch3-SP115973 Well P1-D-09 File SP115973_D009.D Inj Date: 5 May 12 1:33 am - MF C15H16O2 MW 228.1 Expected Conc: 2.97 mM

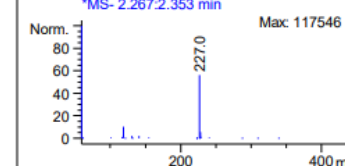
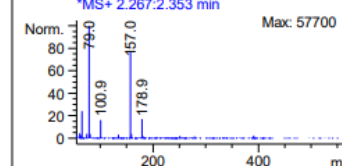
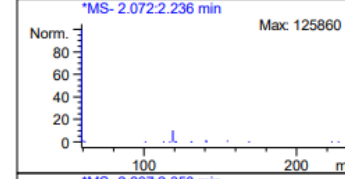
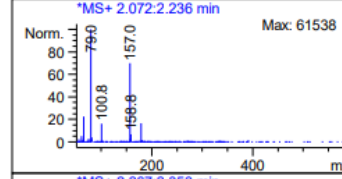
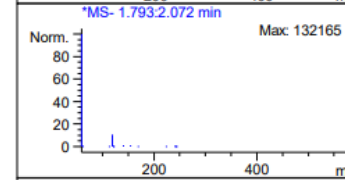
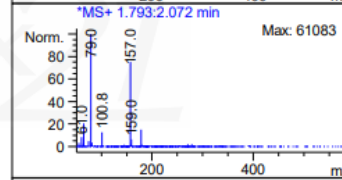
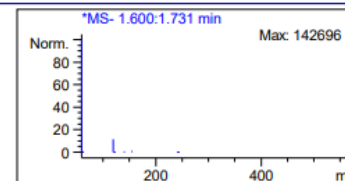
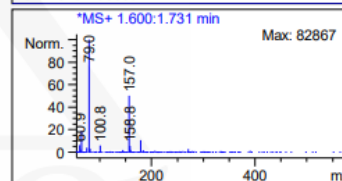


MW Confirmed, Purity>90%

OpAns_Process.MAC Version A.01.10 - Dec 9, 2010

RT	Found	ELS%	UV %	ELS[mg/mL]	Adj [ELS]	[N mM]	Adj [CLN]	#N
1.71		0.0	0.0					0.0
1.84		0.0	0.0					0.0
2.09		0.0	0.0					0.0
2.27	Yes	100.0	100.0	1.76	7.73 mM			0.0

Comment: Passed



Names and CASRNs to Support Searches



United States Environmental Protection Agency

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Search all data

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

▶ LITERATURE

LINKS

COMMENTS

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

25▼

Search query

Synonym	Quality
Bisphenol A	Valid
4,4'-(Propane-2,2-diyl)diphenol	Valid
Phenol, 4,4'-(1-methylethylidene)bis-	Valid
80-05-7 Active CAS-RN	Valid
BPA	Valid
4,4'-Propane-2,2-diylidiphenol	Valid
Phenol, 4,4'-(1-methylethylidene)bis-	Valid
4-06-00-06717 Beilstein Registry Number	Beilstein
(4,4'-Dihydroxydiphenyl)dimethylmethane	Good
2,2-Bis(4'-hydroxyphenyl) propane	Good
2,2'-Bis(4-hydroxyphenyl)propane	Good
2,2-BIS-(4-HYDROXY-PHENYL)-PROPANE	Good
2,2-Bis(4-hydroxyphenyl)propane	Good
2,2-Bis(p-hydroxyphenyl)propane	Good
2,2-Di(4-Hydroxyphenyl) Propane	Good

Literature Searches - Querying 28 Million PubMed abstracts

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

[DETAILS](#)

[EXECUTIVE SUMMARY](#)

[PROPERTIES](#)

[ENV. FATE/TRANSPORT](#)

LITERATURE

[GOOGLE SCHOLAR](#)

PUBMED ABSTRACT SIFTER

[PUBCHEM ARTICLES](#)

[PUBCHEM PATENTS](#)

[PPRTV](#)

[IRIS](#)

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

Optionally, edit the query before retrieving.

"80-05-7" OR "Bisphenol A"

Abstract Sifter - Querying 28 Million PubMed abstracts

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

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EXECUTIVE SUMMARY

PROPERTIES

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HAZARD

ADME

EXPOSURE

BIOACTIVITY

GENRA (BETA)

SIMILAR COMPOUNDS

RELATED SUBSTANCES

SYNONYMS

LITERATURE

GOOGLE SCHOLAR

PUBMED ABSTRACT SIFTER

PUBCHEM ARTICLES

PUBCHEM PATENTS

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

Hazard

Retrieve Articles

118 of 118 articles loaded...

To find articles quickly, enter terms to sift abstracts.

Optionally, edit the query before retrieving.

("80-05-7" OR "Bisphenol A") AND (NOAEL or NOEL OR LOEL or Rfd OR "reference dose" OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])

Download / Send to...

Download Sifter for Excel

<input type="checkbox"/>	PMID	Year	Title	Authors	Journal	Rev
<input type="checkbox"/>	29573712	2018	Urinary bisphenol analogues and triclosan in children from south China and implications f...	Chen; Fang; Ren; Fan; Zhang; Liu; Zhou; Chen; Yu;...	Environmental pollution (Barking, Essex : 1987)	
<input type="checkbox"/>	29306804	2018	Phosphorus flame retardants and Bisphenol A in indoor dust and PM2.5 in kindergartens ...	Deng; Li; Wu; Richard; Wang; Ho	Environmental pollution (Barking, Essex : 1987)	
<input type="checkbox"/>	29268159	2017	Presence of diphenyl phosphate and aryl-phosphate flame retardants in indoor dust from ...	Björnsdotter; Romera-García; Borrull; de Boer; Rubi...	Environment international	
<input type="checkbox"/>	29172986	2017	Bisphenol A and Bisphenol S release in milk under household conditions from baby bottle...	Russo; Barbato; Cardone; Fattore; Albrizio; Grumetto	Journal of environmental science and health. Part. ...	
<input type="checkbox"/>	29097150	2017	Prenatal bisphenol A (BPA) exposure alters the transcriptome of the neonate rat amygdal...	Arambula; Jima; Patisaul	Neurotoxicology	
<input type="checkbox"/>	28982642	2017	Systematic Review and Meta-Analysis of Early-Life Exposure to Bisphenol A and Obesity...	Wassenaar; Trasande; Legler	Environmental health perspectives	✓
<input type="checkbox"/>	28890130	2017	Effects of perinatal bisphenol A exposure on the volume of sexually-dimorphic nuclei of ju...	Arambula; Fuchs; Cao; Patisaul	Neurotoxicology	
<input type="checkbox"/>	28641706	2017	Delayed onset of puberty in male offspring from bisphenol A-treated dams is followed by t...	Oliveira; Romano; de Campos; Cavallin; Oliveira; R...	Reproduction, fertility, and development	
<input type="checkbox"/>	28608465	2017	Effect of bisphenol A on reproductive processes: A review of in vitro, in vivo and epidemiol...	Tomza-Marciniak; Stępkowska; Kuba; Pilarczyk	Journal of applied toxicology : JAT	✓
<input type="checkbox"/>	28503266	2017	Inhalation Toxicity of Bisphenol A and Its Effect on Estrous Cycle, Spatial Learning, and M...	Chung; Han; Lee; Lee	Toxicological research	
<input type="checkbox"/>	28377091	2017	Derivation of an oral Maximum Allowable Dose Level for Bisphenol A.	Goodman; Peterson; Hixon; Pacheco Shubin	Regulatory toxicology and pharmacology : RTP	✓
<input type="checkbox"/>	28257732	2017	Bisphenol A release from orthodontic adhesives measured in vitro and in vivo with gas ch...	Moreira; Matos; de Souza; Brigante; Queiroz; Roma...	American journal of orthodontics and dentofacial ort...	
<input type="checkbox"/>	28219029	2017	Versatile transduction scheme based on electrolyte-gated organic field-effect transistor us...	Piro; Wang; Benaoudia; Tibaldi; Anquetin; Noël; Rei...	Biosensors & bioelectronics	

Relationships in the data

Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by Synonym from Valid Source.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

COMMENTS

12 chemicals

Download / Send

Show info:

DTXSID

CASRN

Select all

Sort by: Relationship

Filter by: Name or CASRN

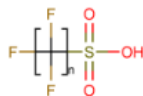
Hide

Searched Chemical



Perfluorooctanesulfonic acid
DTXSID: DTXSID3031864
CASRN: 1763-23-1

Markush Parent



Perfluoroalkyl sulfonates
DTXSID: DTXSID70892979
CASRN: NOCAS_892979

Predecessor: Component

3 related chemical
structures with this
substance

Mixture of PFOS and PFOA
DTXSID: DTXSID20872983
CASRN: NOCAS_872983

Predecessor: Component

3 related chemical
structures with this
substance

1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5...
DTXSID: DTXSID40880545
CASRN: 84202-77-3

Component



Perfluorooctanesulfonate
DTXSID: DTXSID80108992
CASRN: 45298-90-6

Salt Form



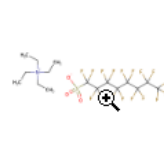
Potassium perfluorooctanesulfonate
DTXSID: DTXSID8037706
CASRN: 2795-39-3

Salt Form



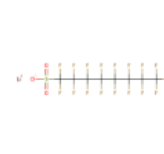
Ammonium perfluorooctanesulfonate
DTXSID: DTXSID9097435
CASRN: 29081-56-9

Salt Form



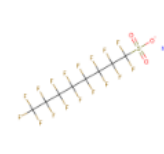
Tetraethylammonium perfluorooctanes...
DTXSID: DTXSID6089128
CASRN: 56773-42-3

Salt Form



Lithium perfluorooctanesulfonate
DTXSID: DTXSID2032421
CASRN: 29457-72-5

Salt Form



Sodium perfluorooctanesulfonate
DTXSID: DTXSID60635462
CASRN: 4021-47-0

Transformation Products

Chlorothalonil

1897-45-6 | DTXSID0020319

Searched by DSSTox Substance Id.

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EXECUTIVE SUMMARY

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EXPOSURE

BIOACTIVITY

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SYNONYMS

LITERATURE

LINKS

COMMENTS

8 chemicals

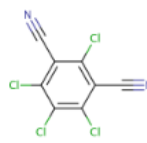
Download / Send

Sort by: Relationship

Show info: DTXSID CASRN Select all

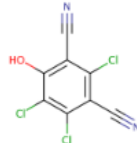
Filter by: Name or CASRN Hide

Searched Chemical



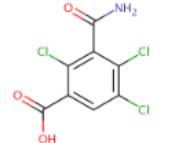
Chlorothalonil
DTXSID: DTXSID0020319
CASRN: 1897-45-6

Transformation Product



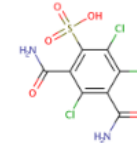
4-Hydroxy-2,5,6-trichloroisophthalonitrile
DTXSID: DTXSID00182588
CASRN: 28343-81-5

Transformation Product



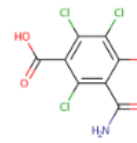
3-Carbamoyl-2,4,5-trichlorobenzoic acid
DTXSID: DTXSID10597537
CASRN: 142733-37-7

Transformation Product



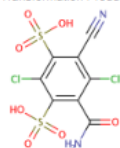
2,4-dicarbamoyl-3,5,6-trichlorobenzene-1-sulfonamide
DTXSID: DTXSID30891327
CASRN: NOCAS_891327

Transformation Product



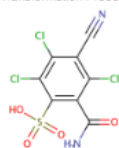
3-carbamoyl-2,5,6-trichloro-4-hydroxybenzoic acid
DTXSID: DTXSID00891328
CASRN: NOCAS_891328

Transformation Product



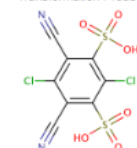
4-carbamoyl-2,5-dichloro-6-cyanobenzene-1-sulfonamide
DTXSID: DTXSID00891329
CASRN: NOCAS_891329

Transformation Product



2-carbamoyl-3,5,6-trichloro-4-cyanobenzene-1-sulfonamide
DTXSID: DTXSID00891330
CASRN: NOCAS_891330

Transformation Product



2,5-dichloro-4,6-dicyanobenzene-1,3-disulfonamide
DTXSID: DTXSID20891331
CASRN: NOCAS_891331

7 salt forms of PFOS (and the ion itself)

Component



Perfluorooctanesulfonate

DTXSID: DTXSID80108992
CASRN: 45298-90-6

Salt Form



Potassium perfluorooctanesulfonate

DTXSID: DTXSID8037708
CASRN: 2795-39-3

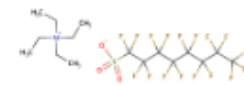
Salt Form



Ammonium perfluorooctanesulfonate

DTXSID: DTXSID9087435
CASRN: 29081-56-9

Salt Form



Tetraethylammonium perfluorooctanesu...

DTXSID: DTXSID5069128
CASRN: 56773-42-3

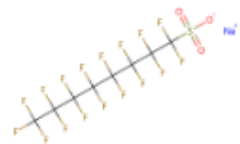
Salt Form



Lithium perfluorooctanesulfonate

DTXSID: DTXSID2032421
CASRN: 29457-72-5

Salt Form



Sodium perfluorooctanesulfonate

DTXSID: DTXSID50635462
CASRN: 4021-47-0

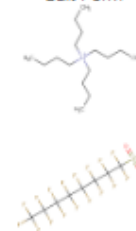
Salt Form



Magnesium bis(perfluorooctane...

DTXSID: DTXSID80881314
CASRN: 91036-71-4

Salt Form



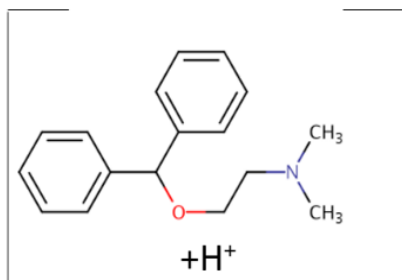
Tetrabutylammonium perfluorooctanesu...

DTXSID: DTXSID40584995
CASRN: 111873-33-7

Using data relationships

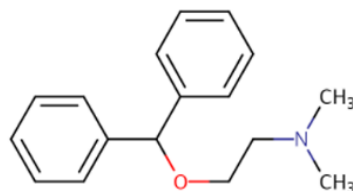
- We have purposely built relationships in the data. Specifically, “MS-Ready mappings”

A) Molecular Ion



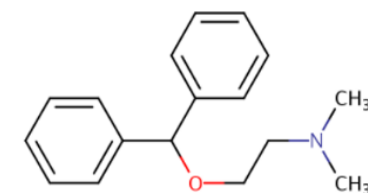
$m/z \approx 256.1702$

B) MS-Ready Form

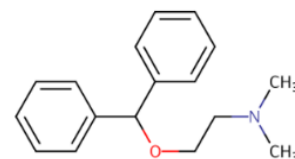


monoisotopic mass= 255.1623
 $C_{17}H_{21}NO$
DTXCID802949

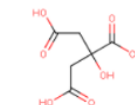
C) Mappings from MS-Ready



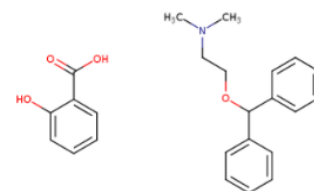
Diphenhydramine
 $C_{17}H_{21}NO$ | 255.1623
DTXCID4022949



Diphenhydramine
hydrochloride
 $C_{17}H_{22}ClNO$ | 291.1390
DTXCID4020537



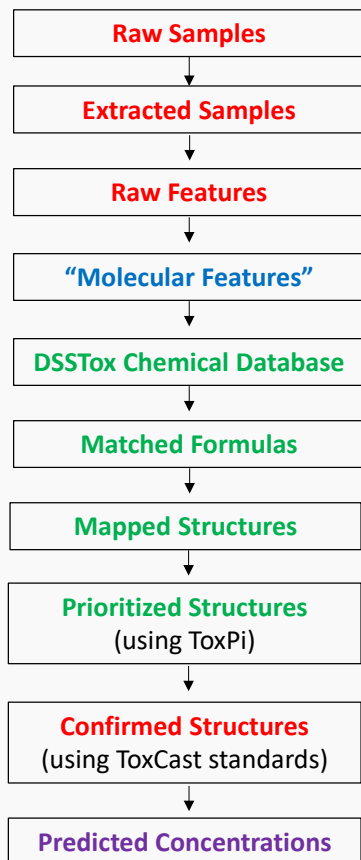
Diphenhydramine citrate
 $C_{23}H_{29}NO_8$ | 447.1893
DTXSID80237211



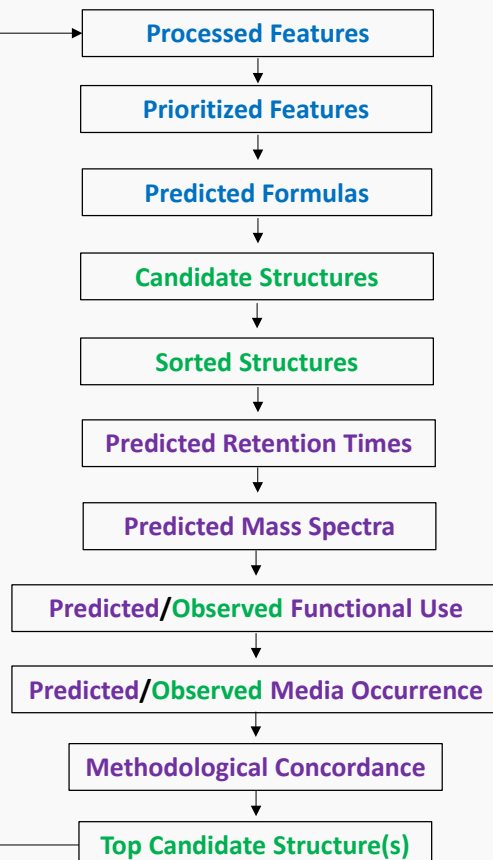
Diphenhydramine salicylate
 $C_{24}H_{27}NO_4$ | 393.1940
DTXSID10225883

“MS-Ready” : Suspect Screening and Non-Targeted Analysis Workflow

Suspect Screening



Non-Targeted Analysis



Color Key

Red = Analytical Chemistry

Blue = Data Processing & Analysis

Purple = Mathematical & QSPR Modeling

Green = Informatics & Web Services



- Singleton searches are useful but we need to search thousands of masses, formulae, names, InChIs and CASRNs!
- Typical questions
 - What chemicals can I get for 5000 CAS Numbers?
 - Can I get predicted properties for 1000 chemicals?
 - What is the list of chemicals for the formula $C_xH_yO_z$?
 - What is the list of chemicals for a mass +/- error ?
 - Can I get chemical lists in Excel files? In SDF files?

Batch Search?



Step Three: Select Download Data or Display Chemicals

Please enter one identifier per line



Select Input Type(s)

☐ Identifiers

☐ Chemical Name 

☐ CASRN 

☐ InChIKey 

☐ DSSTox Substance ID 

☐ InChIKey Skeleton 

☐ MS-Ready Formula(e) 

☐ Exact Formula(e) 

☐ Monoisotopic Mass


Chemical Data


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

Fuel oil, no. 1
Ethylene oxide
Chloromethane
1-Chloropropan-2-one
n-Hexane
Ammonia
Nickel carbonyl
Phosgene
Potassium cyanide
Chlorodimethylsilane

Batch Searching

Select Output Format:






 Excel 

 Download






Customize Results

- ☐ Select All
- ☐ Select All in Lists






Chemical Identifiers

- ☒ DTXSID 
- ☒ Chemical Name 
- ☐ 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 

Presence in Lists:

- ☐ ICCVAM test method evaluation report: in vitro ocular toxicity test methods
- ☐ 40CFR355
- ☐ A list of all PBDEs (Polybrominated diphenyl ethers)
- ☐ A list of all PCBs (Polychlorinated biphenyls)
- ☐ A list of polycyclic aromatic hydrocarbons
- ☐ Acute exposure guideline levels
- ☐ Algal Toxins
- ☐ Androgen Receptor Chemicals
- ☐ APCRA Chemicals for Prospective Analysis
- ☐ APCRA Chemicals for Retrospective Analysis
- ☐ APCRA Chemicals for Retrospective Analysis_App_List_448_Chemicals
- ☐ ATSDR Minimal Risk Levels (MRLs) for Hazardous Substances
- ☐ ATSDR Toxic Substances Portal Chemical List
- ☐ Bisphenol Compounds
- ☐ California Office of Environmental Health Hazard Assessment
- ☐ Chemicals with interesting names
- ☐ CMAP
- ☐ DNT Screening Library
- ☐ Drinking Water Suspects, KWR Water, Netherlands
- ☐ EDSP Universe
- ☐ EPA Chemicals associated with hydraulic fracturing
- ☐ EPA Chemicals associated with hydraulic fracturing

Excel Output

	A	B	C	D	E	F	G	H
1	INPUT	FOUND_BY	DTXSID	PREFERRED_NAME	EXPOCAS1	EXPOCAS1	NHANES	TOXVAL_D
2	1445-75-6	CAS-RN	DTXSID5024051	Diisopropyl methylphosphonate	2.09e-08	Y	-	Y
3	50-00-0	CAS-RN	DTXSID7020637	Formaldehyde	1.32e-06	Y	-	Y
4	107-06-2	CAS-RN	DTXSID6020438	1,2-Dichloroethane	4.9e-06	Y	-	Y
5	57-12-5	CAS-RN	DTXSID6023991	Cyanide	-	-	-	Y
6	7550-45-0	CAS-RN	DTXSID8042476	Titanium tetrachloride	-	-	-	Y
7	79-01-6	CAS-RN	DTXSID0021383	Trichloroethylene	7.27e-06	Y	-	Y
8	121-82-4	CAS-RN	DTXSID9024142	Cyclonite	6.72e-08	Y	-	Y
9	108-05-4	CAS-RN	DTXSID3021431	Vinyl acetate	8.3e-05	Y	-	Y
10	7803-51-2	CAS-RN	DTXSID2021157	Phosphine	-	-	-	Y
11	122-66-7	CAS-RN	DTXSID7020710	1,2-Diphenylhydrazine	1.49e-07	Y	-	Y
12	101-77-9	CAS-RN	DTXSID6022422	4,4'-Methylenedianiline	6.08e-06	Y	-	Y
13	14017-34-6	CAS-RN	DTXSID90161250	Selenium difluoride	-	-	-	-
14	75-44-5	CAS-RN	DTXSID0024260	Phosgene	-	-	-	Y
15	621-64-7	CAS-RN	DTXSID6021032	N-Nitrosodipropylamine	4.55e-07	Y	-	Y
16	75-09-2	CAS-RN	DTXSID0020868	Dichloromethane	2.02e-06	Y	-	Y
17	100-41-4	CAS-RN	DTXSID3020596	Ethylbenzene	8.32e-05	Y	-	Y
18	7440-28-0	CAS-RN	DTXSID2036035	Thallium	-	-	-	Y
19	108-88-3	CAS-RN	DTXSID7021360	Toluene	8.61e-05	Y	-	Y
20	111-44-4	CAS-RN	DTXSID9020168	Bis(2-chloroethyl) ether	2.82e-07	Y	-	Y
21	7440-42-8	CAS-RN	DTXSID3023922	Boron	-	-	-	Y
22	7440-29-1	CAS-RN	DTXSID6049800	Thorium	-	-	-	Y

List of Chemicals

Lists of Chemicals

List of Assays

Select List

Show 10 entries

Search:

Download

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
40CFR355	40CFR355	2018-01-05	354	Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378)
AEGLVALUES	Acute exposure guideline levels	2018-04-20	174	Acute exposure guideline levels (AEGLs) describe the human health effects from once-in-a-lifetime, or rare, exposure to airborne chemicals.
ALGALTOX	Algal Toxins	2017-11-21	54	A set of algal toxins of interest
APCRA_PRO	APCRA Chemicals for Prospective Analysis	2018-02-14	204	The APCRA prospective case study list of approximately 200 chemicals as of January 2018, developed by ECHA in consultation with EPA and other partners
APCRA_RETRO	APCRA Chemicals for Retrospective Analysis	2018-02-14	380	The APCRA retrospective case study list of 380 chemicals that have ToxCast/Tox21 data, httk, and point-of-departure values that meet case study criteria in ToxValDB.
APCRAAPPLIST	APCRA Chemicals for Retrospective Analysis_App_List_448_Chemicals	2018-05-23	447	The APCRA retrospective case study list of 380 chemicals that have ToxCast/Tox21 data, httk, and point-of-departure values that meet case study criteria in ToxValDB. This is the EDITABLE app list
ARCHEMICALS	Androgen Receptor Chemicals	2018-05-01	110	The list of chemicals used to identify references with in vitro AR binding . From Kleinstreuer et al http://pubs.acs.org/doi/abs/10.1021/acs.chemrestox.6b00347
ATHENSSUS	University of Athens Surfactant and Suspect List	2017-07-14	60	ATHENSSUS is a compilation of suspects, predicted transformation products and surfactants screened in wastewater by University of Athens, as described in Gago-Ferrero et al 2015, DOI: 10.1021/acs.est.5b03454
comptox-prod.epa.gov/dashboard/chemical_lists	ATSDR List	2017-03-11	200	The Agency for Toxic Substances and Disease Registry (ATSDR) is a federal public health

EPA activities around PFAS chemicals

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

Per- and Polyfluoroalkyl Substances (PFAS)

CONTACT US

SHARE



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](#)

The OECD List of PFAS

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



Port

HOME



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.



INARS



11 PFAS Lists

http://comptox-prod.epa.gov/dashboard/chemical_lists

Select List

Show 10 entries

Search: pfas

Download

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
EPAPFAS75S1	EPA PFAS 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.
EPAPFASCAT	Registered DSSTox "category substances" representing Per- and Polyfluoroalkyl Substances (PFAS) 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 in EPA's 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 in EPA's ToxCast Chemical Inventory	2018-06-29	430	PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing.
EPAPFASRL	EPA PFAS Cross-Agency Research List	2018-07-27	194	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.
PFASEPA	PFAS_EPA List of Perfluorinated alkyl substances	2017-11-03	190	PFAS_EPA (Perfluorinated alkyl substances) is a manually curated listing of mainly straight-chain and branched PFAS substances
PFASEUOECD	PFAS Listed in OECD Global Database	2018-07-26	4725	OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances, (PFASs) listing approximately 4700 new PFAS
PFASGRACE	PFASforGrace	2017-02-16	35	A list of polyfluorinated chemicals of interest to Grace Patlewicz
PFASKEMI	PFAS List from the Swedish Chemicals Agency (KEMI) Report	2017-02-09	2397	Perfluorinated substances from a Swedish Chemicals Agency (KEMI) Report on the occurrence and use of highly fluorinated substances.
PFASMASTER	PFAS Master List of PFAS Substances	2018-07-26	5061	PFASMASTER is a consolidated list of PFAS substances spanning and bounded by the below lists of current interest to researchers and regulators worldwide.

Showing 1 to 10 of 11 entries (filtered from 96 total entries)

PFAS Categories in Development

Registered DSSTox “category substances” representing Per- and Polyfluoroalkyl Substances (PFAS) categories

Q

☐ 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 is undergoing continuous curation and expansion.

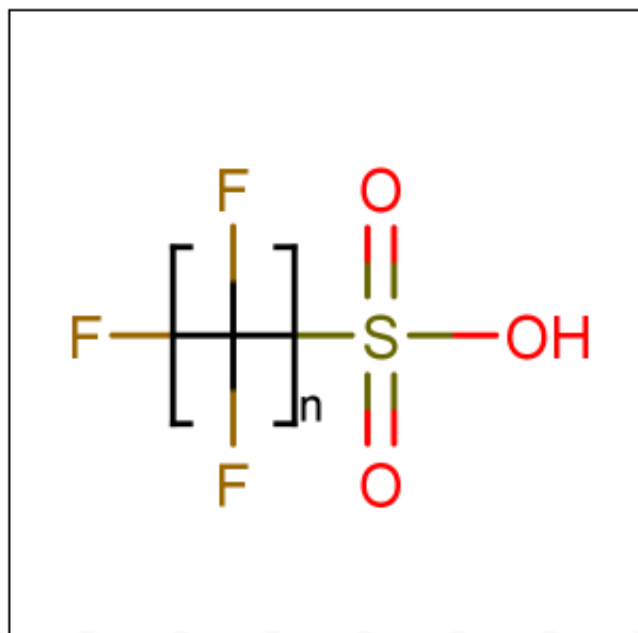
Number of Chemicals: 64

- PFOS is a member of linear perfluoroalkyl sulfonates

Perfluoroalkyl sulfonates

NOCAS_892979 | DTXSID70892979

Searched by DSSTox Substance Id.



- Mapping between our data (and websites) has resulted in collaborative data curation
- Collaboration with Emma Schymanski re. the NORMAN Suspects Exchange
<https://www.norman-network.com/?q=node/236>
- Multiple NORMAN lists now mapped

NORMAN Suspect Exchange

NORMAN

Network of reference laboratories, research centres and related organisations for monitoring of emerging environmental substances

[Home](#) | [NORMAN Network](#) | [Working Groups](#) | [Membership](#) | [NORMAN Bulletin](#) | [Success Stories](#) | [Publications](#) | [Job opportunities](#) | [Contact](#) | [Gallery](#) | [Members' Area](#) | [NORMAN GA meetings](#)

Menu

- Emerging Substances
- DATABASES
- Topics and Activities
- Workshops and Events
- QA/QC Issues
- Glossary
- Useful links
- Members' Area

User login

Username *

Password *

[Request new password](#)

Home

<http://www.norman-network.com/?q=node/236>

NORMAN Suspect List Exchange

In September 2014, NORMAN members expressed the need to exchange various lists of substances to improve their suspect screening efforts. This website was established as part of the 2015 Joint Programme of Activities as a central access point for NORMAN members (and others) to find suspect lists relevant for their environmental monitoring question. All suspect lists currently available are compiled in the table below and on the US EPA CompTox Chemistry Dashboard ([website](#), [downloads](#), [chemical lists](#)).

The "Link to full list" column below contains an excel or comma-separated file (csv) with all available information, e.g. as provided as supporting information for the publication, while the third column provides a list of the structures as InChIKeys only, which allows suspect searching using MetFrag or other workflows. The fourth column contains references for the data: please cite these references if you use the respective datasets.

Recent Suspect Exchange and Dashboard presentations/publications include: **ICCE Oslo 2017: NORMAN Suspects meet the Dashboard** and **NORMAN MassBank and Suspect Exchange**; SETAC Mixtures Denver: **Identifying Complex Mixtures with Cheminformatics and HR-MS**; ACS Fall 2017: **Markush Enumeration for UVCBs** and a [viewpoint article](#).

No.	Abbreviation	Description	Link to full list	Link to InChIKey list	References
	SUSDAT	Merged NORMAN Suspect List: SusDat	Interactive Data table (updating...)	MS-ready InChIKeys (1/03/2018)	A merged list of >40,000 structures from suspect lists. See interactive version . Compiled by Reza Aalizadeh, University of Athens, including RTI and toxicity values, support by Nikiforos Alygizakis, EI. <i>Work in progress ... please report any issues!</i>
S1	MASSBANK	NORMAN Compounds in MassBank	CSV, XLSX with Fragments (3/10/2017) CompTox MassBank EU Reference List CompTox MassBank EU Special Cases CompTox Fragment Download	MassBankEUInChIKeys (11/04/2017)	www.massbank.eu Stravs <i>et al.</i> 2013. DOI: 10.1002/jms.3131
S2	STOFFIDENT	HSWT/LfU STOFF-IDENT Database of Water-Relevant Substances	STOFF-IDENT Contents (6/09/2017) CompTox STOFF-IDENT List Further curation in progress...	STOFF-IDENT InChIKeys (6/09/2017)	The database enables the search for exact masses from target or unknown lists and the automatic use of a Retention Time Index. See: https://www.lfu.bayern.de/stoffident/#!home (single search for free; batch search after free registration).
S3	NORMANCT15	NORMAN Collaborative Trial Targets and Suspects	LC-MS: CSV, XLSX (3/10/2017) GC-MS: CSV, XLSX (3/10/2017) CompTox NORMANCT15 List	LC-MS InChIKeys (31/10/2016) GC-MS InChIKeys (31/10/2016)	Schymanski <i>et al.</i> 2015. DOI: 10.1007/s00216-015-8681-7

Example: NORMAN Priority List

S15	NORMANPRI	NORMAN Priority List	NORMAN Priority CSV (13/7/2017) CompTox NORMAN Priority List Further curation in progress...	NORMAN Priority InChIKeys (16/05/2017)	Priority substances from NORMAN WG-1 (Prioritisation), provided by Valeria Dulio.
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← → ↻ 🏠 https://comptox.epa.gov/dashboard/chemical_lists/norman 80% ⋮ ☆ 🔍 Search

EPA United States Environmental Protection Agency Home Advanced Search Batch Search Lists ▾ Predictions Downloads Share 🔍 Search all data

NORMAN Network Priority List

Search NORMANPRI Chemicals 🔍

☐ Substring search

List Details

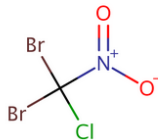
Description: NORMANPRI contains the list of priority substances determined by the NORMAN Network [Working Group 1](#) on Prioritization, provided by Valeria Dulio, INERIS, France. Further details are available on the Working Group website. The original data is available on the [NORMAN Suspect List Exchange](#). This list is undergoing continuous curation/extension.

Number of Chemicals: 922

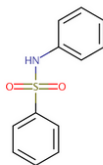
922 chemicals

Download / Send ▾ Show info: DTXSID ✕ CASRN ✕ TOXCAST ✕ Select all 📄

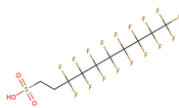
Sort by: DTXSID ⬆️ Filter by: Name or CASRN Hide ▾



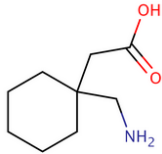
Dibromochloronitromethane
DTXSID:DTXSID00152114
CASRN:1184-89-0
TOXCAST:0



Benzenesulfonanilide
DTXSID:DTXSID00168371
CASRN:1678-25-7
TOXCAST:0

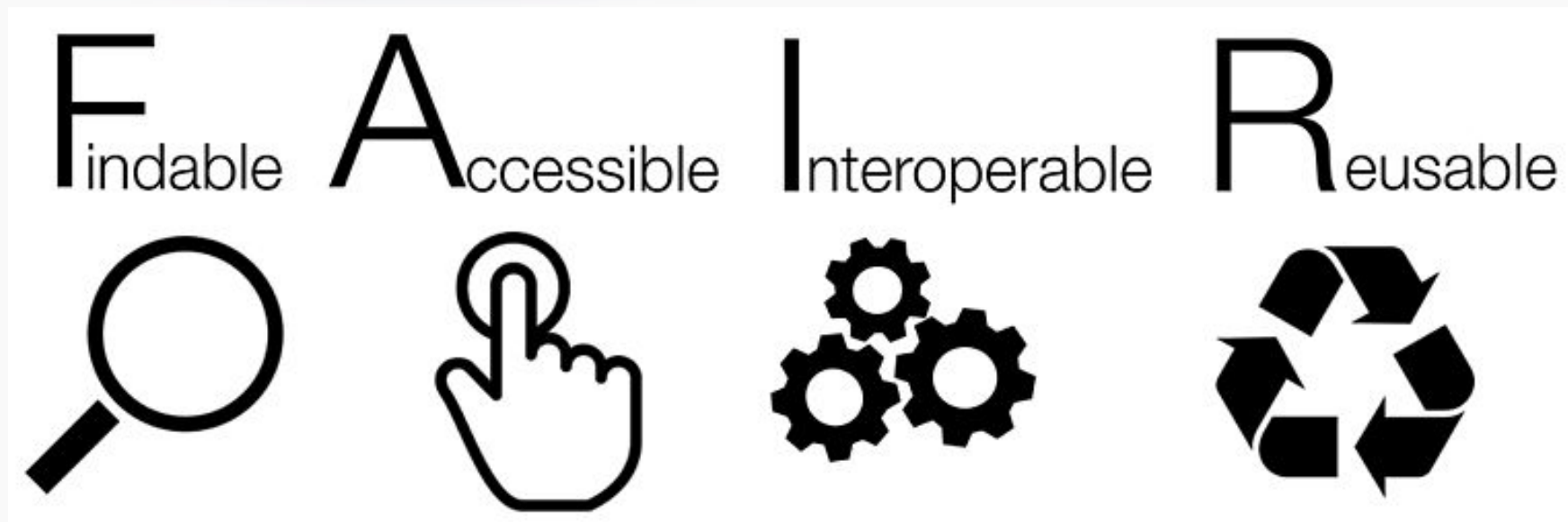


8:2 Fluorotelomer sulfonic acid
DTXSID:DTXSID00192353
CASRN:39108-34-4
TOXCAST:0



Gabapentin
DTXSID:DTXSID0020074
CASRN:60142-96-3
TOXCAST:0

Our support for FAIR Data



- We're definitely not there yet...but are making progress at speed...

- Our data are licensed as public domain data
 - available from downloads page
 - registered to Figshare
 - SQL data dumps
- Collection of web services for old dashboards are available – API is being fully revamped

API in development

Prototype services available

<https://comptox.epa.gov/dashboard/web-test/WS?smiles=CCO&method=hc>

JSONRaw DataHeaders

SaveCopy

uuid:"55547f4f-f966-48e8-b831-a0d217998064"

predictionTime:1520539090089

software:"T.E.S.T (Toxicity Estimation Software Tool)"

softwareVersion:"5.01"

condition:"25°C"

endpoint:"Water solubility at 25°C"

method:"Hierarchical clustering"

▼ predictions:

▼ 0:

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smiles:"OCC"

expValMolarLog:"-1.337"

expValMass:"1001180.703"

predValMolarLog:"-1.338"

predValMass:"1002625.241"

molarLogUnits:"-Log10(mol/L)"


massUnits:"mg/L"

How we are serving FAIR

- Our data are licensed as public domain data
 - available from downloads page
 - registered to Figshare
 - SQL data dumps
- Collection of web services for old dashboards are available – API is being fully revamped
- Models are published to Github

OPERA Models on Github

<https://github.com/kmansouri>



Kamel Mansouri
kmansouri

- Computational Chemistry/Toxicology -
Cheminformatics and data mining -
QSAR/QSPR and ADME-Tox properties modeling [orcid:0000-0002-6426-8036]

Block or report user

RTP, NC, USA

<https://www.linkedin.com/in/ka...>

Overview Repositories 3 Stars 3 Followers 5 Following 4

Popular repositories

OPERA

Command line application providing QSAR models predictions as well as applicability domain and accuracy assessment for physicochemical properties and environmental fate endpoints.

★ 3 🍴 1

QSAR-ready

Standardization workflow for QSAR-ready chemical structures pretreatment.


MS-ready

Standardization workflow for MS-ready chemical structures pretreatment.

12 contributions in the last year

	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep
Mon												
Wed												
Fri												

[Learn how we count contributions.](#)

Less  More

- The last public release of ToxCast data (invitroDB_v2) was in 3rd Quarter of 2015
- Next release of invitroDB_v3 is Fall 2018
- Data includes new assays, new chemicals, new pipelining, results of data curation
- Data will also release via the Dashboard
- Data available at <https://www.epa.gov/chemical-research/exploring-toxcast-data-downloadable-data>

In Progress: Metabolites extracted from literature and databases

Chlorothalonil

1897-45-6 | DTXSID0020319

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

COMMENTS

8 chemicals

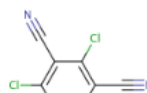
Download / Send

Sort by: Relationship

Show info: DTXSID CASRN Select all

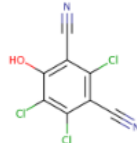
Filter by: Name or CASRN Hide

Searched Chemical



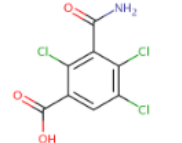
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CASRN: 1897-45-6

Transformation Product



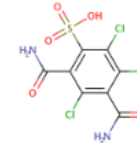
4-Hydroxy-2,5,6-trichloroisophthalonitrile
DTXSID: DTXSID00182588
CASRN: 28343-81-5

Transformation Product



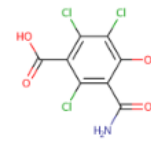
3-Carbamoyl-2,4,5-trichlorobenzoic acid
DTXSID: DTXSID10597537
CASRN: 142733-37-7

Transformation Product



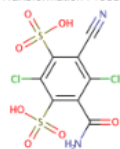
2,4-dicarbamoyl-3,5,6-trichlorobenzene-1-sulfonamide
DTXSID: DTXSID30891327
CASRN: NOCAS_891327

Transformation Product



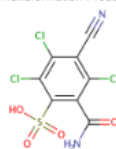
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DTXSID: DTXSID00891328
CASRN: NOCAS_891328

Transformation Product



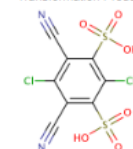
4-carbamoyl-2,5-dichloro-6-cyanobenzene-1-sulfonamide
DTXSID: DTXSID00891329
CASRN: NOCAS_891329

Transformation Product



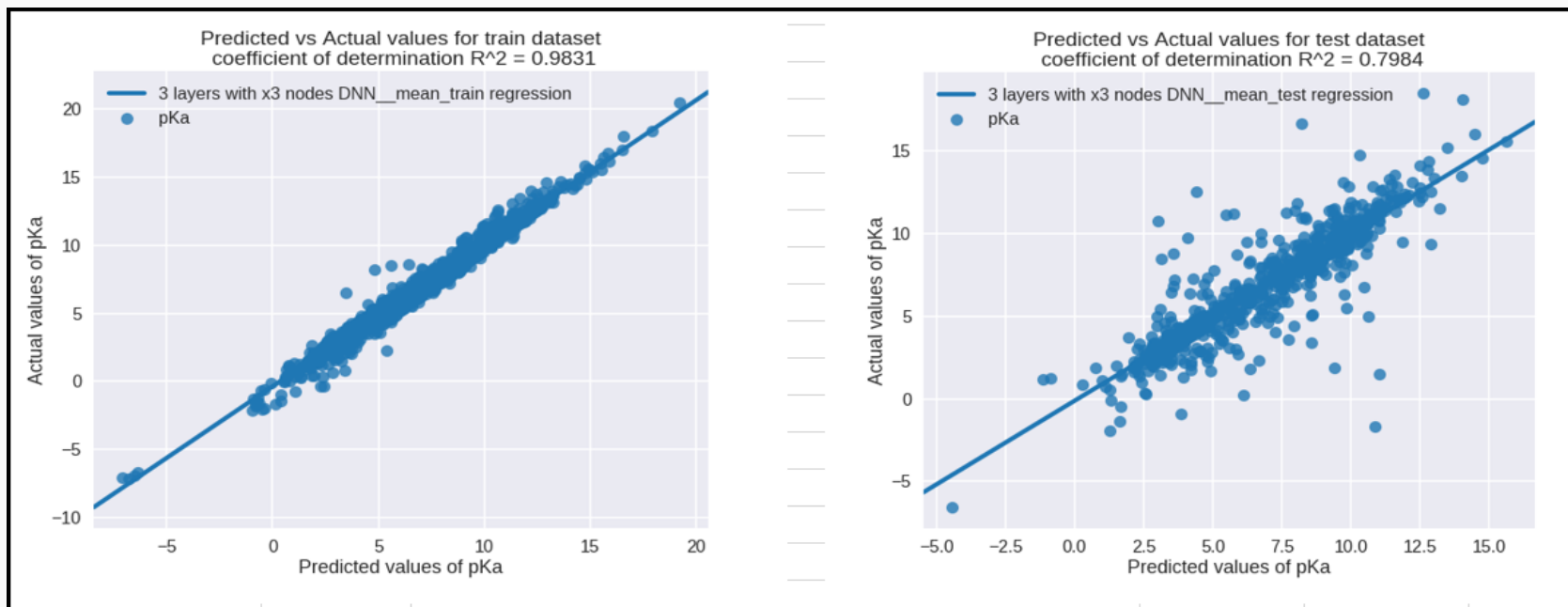
2-carbamoyl-3,5,6-trichloro-4-cyanobenzene-1-sulfonamide
DTXSID: DTXSID00891330
CASRN: NOCAS_891330

Transformation Product



2,5-dichloro-4,6-dicyanobenzene-1,3-disulfonamide
DTXSID: DTXSID20891331
CASRN: NOCAS_891331

- pKa prediction models based on Open Data Set of 8000 chemicals – acidic, basic and amphoteric chemicals

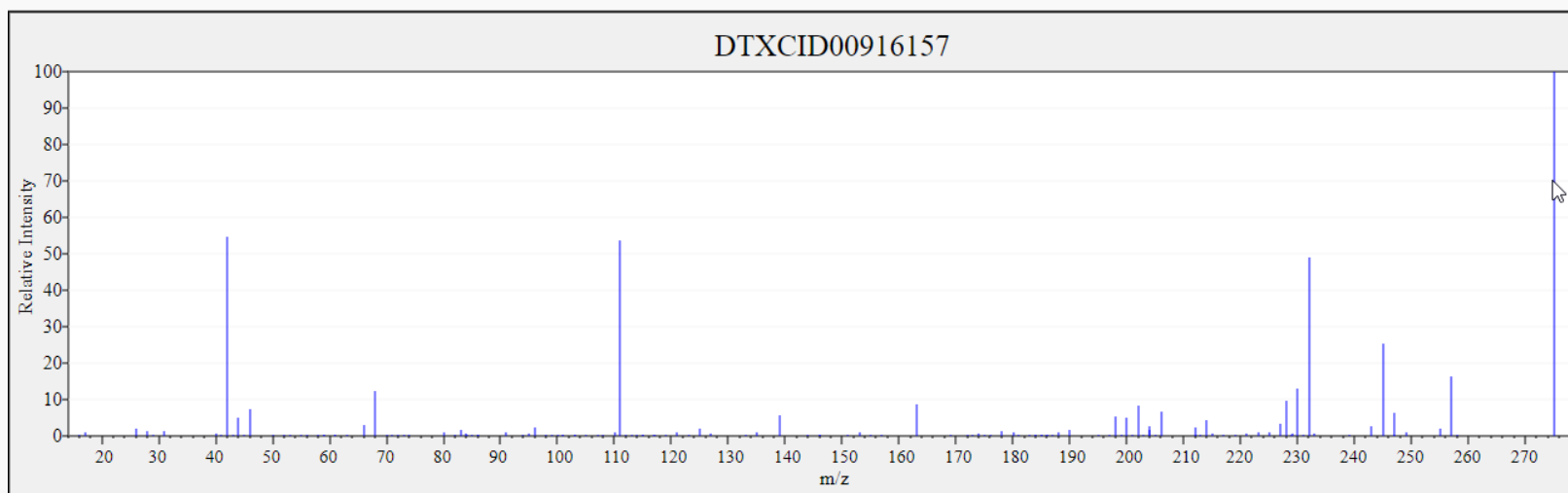


In Progress: 700k Predicted MS

<http://cfmid.wishartlab.com/>

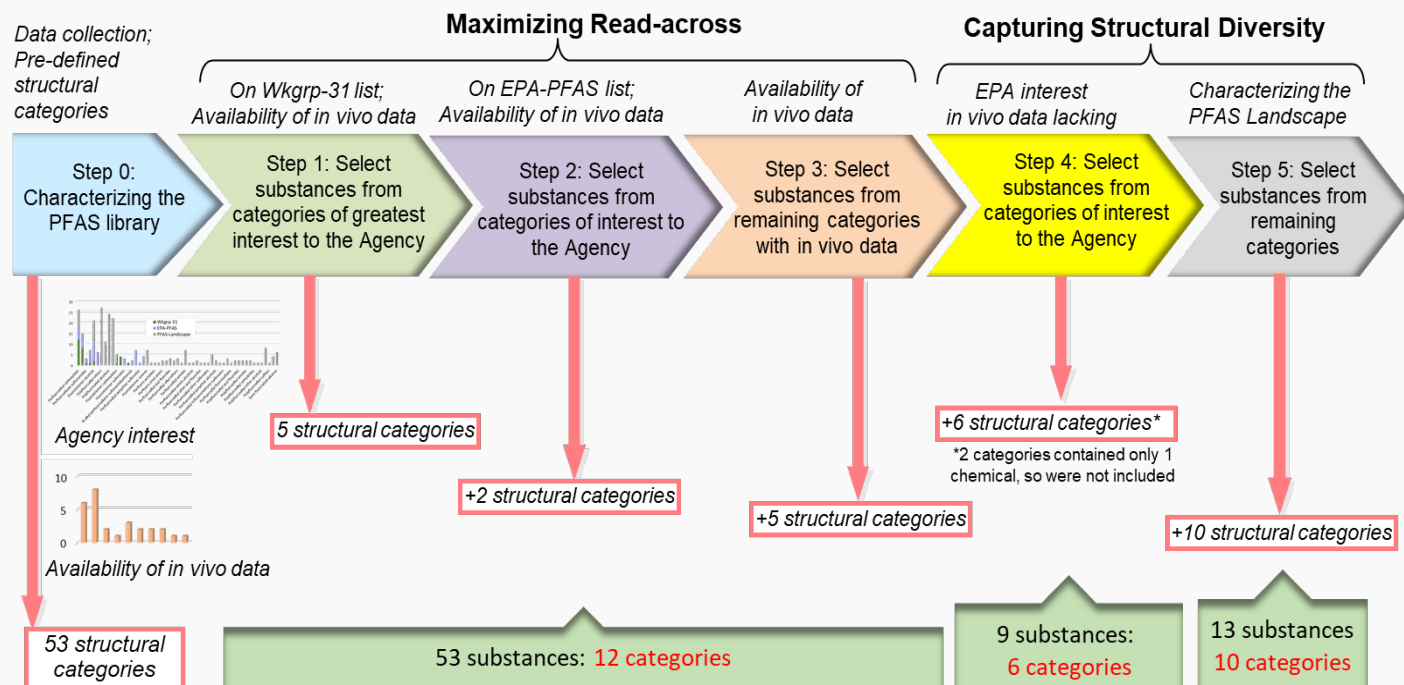


- MS/MS spectra prediction for ESI+, ESI-, and EI
- Predictions generated and stored for >700,000 structures, to be accessible via Dashboard



In progress: PFAS Chemical Library

- Development of a high-throughput screening library and collection of physical samples (~400)
- 75 PFAS chemicals for screening based on categories, diversity, exposure considerations, procurability and testability, availability of existing toxicity data



- Transparent access to data supporting computational toxicology – file downloads, SQL data dumps and web services
- CompTox Chemicals Dashboard provides access to data for ~765,000 chemicals
- Our publications provide chemistry data in usable formats – Excel, SDF (V2000/V3000)
- Web Services developing to serve API development
- Next release: Fall 2018 with InvitroDB_v3 data

Acknowledgements



Credit: the Research Triangle Foundation

EPA-RTP

- *An enormous team of contributors from NCCT, especially the IT software development team*
- *Multiple centers and laboratories across the EPA*
- *Many public domain databases and open data contributors*

Antony Williams

NCCT, US EPA Office of Research and Development,

Williams.Antony@epa.gov

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

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


 Journal of Cheminformatics

DATABASE

Open Access

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



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

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