

Informatics Approaches supporting UVCB Chemicals in the US-EPA CompTox Chemicals Dashboard

Antony Williams¹, Chris Grulke¹ and Emma Schymanski²

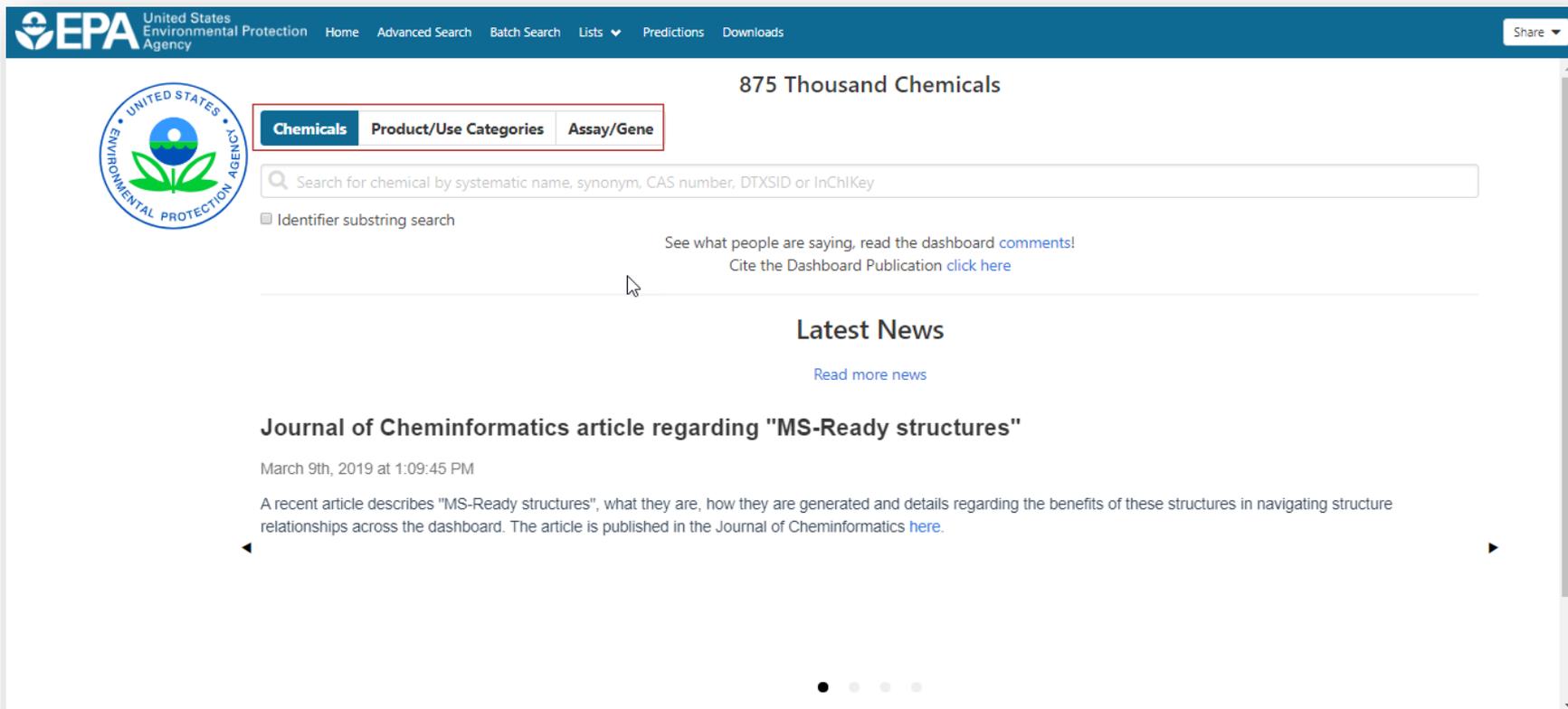
*Center for Computational Toxicology and Exposure, U.S. Environmental Protection Agency, RTP, NC
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The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA

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SETAC, Toronto, Canada*

- The CompTox Chemicals Dashboard - web-based database of 875k substances
- Associated data including:
 - Experimental and predicted physicochemical data
 - *In vivo* hazard data
 - *In vitro* bioactivity screening data
 - Link farm to tens of public resources
- Integrated modules – read-across, lit search
- Data mappings and searches supporting Mass Spectrometry & structure identification

875k Chemical Substances



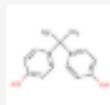
The screenshot displays the EPA CompTox Chemicals Dashboard. At the top, the EPA logo and navigation links (Home, Advanced Search, Batch Search, Lists, Predictions, Downloads) are visible. The main heading is "875 Thousand Chemicals". Below this, there are three tabs: "Chemicals", "Product/Use Categories", and "Assay/Gene". A search bar is present with the placeholder text "Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey". There is also a checkbox for "Identifier substring search". Below the search bar, there are links to "See what people are saying, read the dashboard comments!" and "Cite the Dashboard Publication [click here](#)". The "Latest News" section features an article titled "Journal of Cheminformatics article regarding 'MS-Ready structures'" dated March 9th, 2019 at 1:09:45 PM. The article text states: "A recent article describes 'MS-Ready structures', what they are, how they are generated and details regarding the benefits of these structures in navigating structure relationships across the dashboard. The article is published in the Journal of Cheminformatics [here](#)." Navigation arrows and a progress indicator are visible at the bottom of the news section.

Chemicals

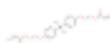
Product/Use Categories

Assay/Gene

 Bisphenol



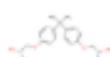
Bisphenol A
DTXSID7020182



Bisphenol A bis(2-hydroxyethyl ether) diacrylate
DTXSID6066991

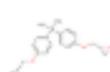


Bisphenol A bis(2-hydroxyethyl ether) dimethacrylate
DTXSID1066992

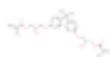


Bisphenol A bis(2-hydroxypropyl) ether
DTXSID8051592

Bisphenol A carbonate polymer
DTXSID6027840



Bisphenol A diglycidyl ether
DTXSID6024624



Bisphenol A glycidyl methacrylate
DTXSID7044841

Detailed Chemical Pages

 United States Environmental Protection Agency

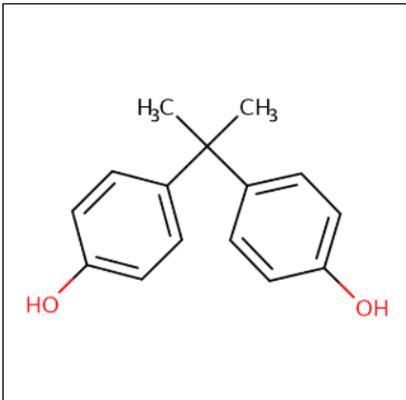
Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search all data

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.



DETAILS

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

Wikipedia

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 (0.344 wt % at 83 °C). BPA is a starting material for the synthesis of plastics, primarily certain polycarbonates

[Read more](#)

Intrinsic Properties

 **Molecular Formula:** $\text{C}_{15}\text{H}_{16}\text{O}_2$  Mol File  Find All Chemicals

 **Average Mass:** 228.291 g/mol  Isotope Mass Distribution

 **Monoisotopic Mass:** 228.11503 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

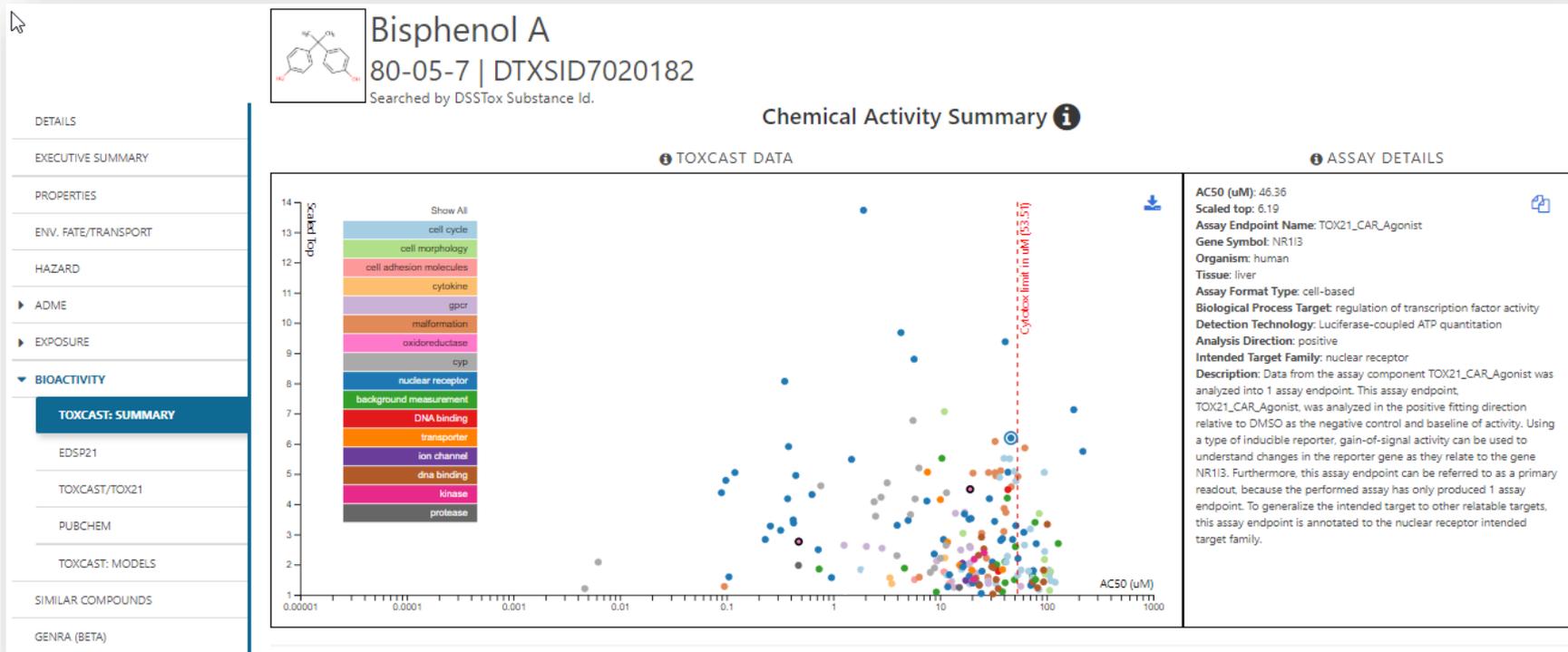
Record Information

Quality Control Notes

- ToxVal Database contains following data:
 - ~700,000 toxicity values
 - ~30 sources of data
 - ~22,000 sub-sources
 - ~5000 journals cited
 - ~70,000 literature citations

In Vitro Bioassay Screening

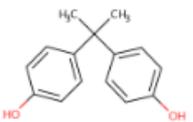
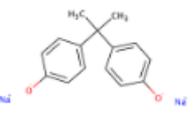
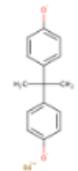
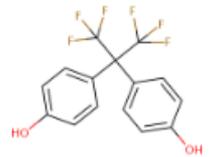
ToxCast and Tox21



Related Substances – Transformation Products, “Monomer-Polymer”

8 chemicals

Select all Download Send to Batch Search Relationship DTXSID PubChem CPDAT Hide chemicals that are: Filter by Name or CASRI

<p>Searched Chemical</p>  <p>Bisphenol A DTXSID: DTXSID7020182 PubChem: 161 CPDAT: 326</p>	<p>Polymer</p> <p>2 related chemical structures with this substance</p> <p>Formaldehyde, polymer with bisphenol A DTXSID: DTXSID3049627 PubChem: 0 CPDAT: 4</p>	<p>Polymer</p> <p>2 related chemical structures with this substance</p> <p>Bisphenol A/ Epichlorohydrin resin DTXSID: DTXSID0050479 PubChem: 0 CPDAT: 531</p>	<p>Polymer</p> <p>3 related chemical structures with this substance</p> <p>Bisphenol A-epichlorohydrin-polyformal... DTXSID: DTXSID9050480 PubChem: 0 CPDAT: 3</p>	<p>Predecessor: Component</p> <p>3 related chemical structures with this substance</p> <p>Bisphenol A-epichlorohydrin-2,2',6,6'-tet... DTXSID: DTXSID70872791 PubChem: 0 CPDAT: 6</p>
<p>Salt Form</p>  <p>Phenol, 4,4'-(1-methylethylidene)bis-, di... DTXSID: DTXSID0027480 PubChem: 21 CPDAT: 1</p>	<p>Salt Form</p>  <p>Barium(2+) 4,4'-isopropylidenebispheno... DTXSID: DTXSID90240211 PubChem: 6 CPDAT: 0</p>	<p>Transformation Product</p>  <p>Bisphenol AF DTXSID: DTXSID7037717 PubChem: 97 CPDAT: 17</p>	<h2>What No Structures???</h2>	

***“UVCB”
Chemical
Substances***

Chemical Substances of Unknown or Variable Composition, Complex Reaction Products and Biological Materials (UVCB Substance) on the TSCA Inventory

This paper is a compendium of information related to the broad class of chemical substances referred to as UVCBs for the Toxic Substances Control Act (TSCA) Chemical Substance Inventory. These chemical substances cannot be represented by unique structures and molecular formulas.

Lots of UVCBS in Commerce....

1 related chemical
structure with this
substance

Butoxypropylene glycol
DTXSID: DTXSID3034404
PubChem: 0
CPDAT: 437

0 related chemical
structures with this
substance

Fatty acids, tall-oil
DTXSID: DTXSID0028088
PubChem: 0
CPDAT: 436



Poly(oxy-1,2-ethanediyl), alpha-tridecyl-...
DTXSID: DTXSID8043993
PubChem: 0
CPDAT: 435

1 related chemical
structure with this
substance

Polyoxyethylene (20) oleylether
DTXSID: DTXSID1027714
PubChem: 0
CPDAT: 435

0 related chemical
structures with this
substance

Soy oil
DTXSID: DTXSID8027660
PubChem: 0
CPDAT: 435

0 related chemical
structures with this
substance

Bentonite
DTXSID: DTXSID6030782
PubChem: 0
CPDAT: 433

0 related chemical
structures with this
substance

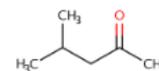
Distillates, petroleum, hydrotreated heav...
DTXSID: DTXSID3028217
PubChem: 0
CPDAT: 433

1 related chemical
structure with this
substance

Edifas B
DTXSID: DTXSID2020555
PubChem: 0
CPDAT: 433

0 related chemical
structures with this
substance

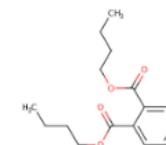
Coconut oil
DTXSID: DTXSID8027664
PubChem: 0
CPDAT: 432



4-Methyl-2-pentanone
DTXSID: DTXSID5021889
PubChem: 173
CPDAT: 428

0 related chemical
structures with this
substance

Distillates, petroleum, solvent-refined he...
DTXSID: DTXSID9028172
PubChem: 0
CPDAT: 426



Dibutyl phthalate
DTXSID: DTXSID2021781
PubChem: 138
CPDAT: 421

- Aroclor 1254
- Toxaphene
- Xylenes
- Demeton
- Aroclor 1248
- Asbestos
- Technical chlordane
- Coke oven emissions
- Creosote
- Diesel engine exhaust
- Nickel refinery dust
- Nickel, soluble salts
- Refractory ceramic fibers
- Toluene diisocyanate

What is Toxaphene?

“Complex, but reproducible mixture of at least **175** distinct C₁₀-chloro compounds, having an approximate overall empirical formula of C₁₀H₁₀Cl₈.; the 2 most active components are a C₁₀H₁₀Cl₈ compound and a C₁₀H₁₁Cl₇ compound which had been elucidated as 2,2,5-endo,6-exo,8,9,10-heptachlorobornane.

Produced by the chlorination of camphene to 67-69% chlorine by weight and made up of compds. of C₁₀ H₈ Cl₁₀, C₁₀ H_{18-n} Cl_n (mostly polychlorobornanes) and C₁₀ H_{16-n} Cl_n (polychlorobornanes and/or polychlorotricyclenes) with n = 6 to 9”

Toxaphene has rich data

8001-35-2 | DTXSID7021368

Searched by DSSTox Substance Id.

Chemical Activity Summary i

Hazard

8001-35-2 | DTXSID7021368

Searched by DSSTox Substance Id.

Toxics Release Inventory

2015 TRI Factsheet: Chemical - TOXAPHENE, 008001352

Data Source: 2018 Updated Dataset (released October 2019)

The [Toxics Release Inventory \(TRI\)](#) tracks the management of certain toxic chemicals that may pose a threat to human health and the environment. Certain industrial facilities in the U.S. must report annually how much of each chemical is recycled, combusted for energy recovery, treated for destruction, and disposed of or otherwise released on- and off-site. This information is collectively referred to as production-related waste managed.

Map of TRI Facilities Reporting TOXAPHENE



Quick Facts for 2015

	Chemical	United States
Number of TRI Facilities:	16	22,286
Total Production-Related Waste Managed:	200.2 thousand lbs	28.9 billion lbs
Total On-site and Off-site Disposal or Other Releases:	15.0 thousand lbs	3.4 billion lbs
Total On-site:	14.0 thousand lbs	2.9 billion lbs
• Air:	25 lbs	690.4 million lbs
• Water:	0 lbs	199.3 million lbs
• Land:	14.0 thousand lbs	2.0 billion lbs
Total Off-site:	1.0 thousand lbs	511.4 million lbs

TOXAPHENE ranks 239 out of 499 chemicals reported to TRI in 2015 (Rank 1 = highest releases)

UVCB: Mapped Chemicals

Polymer individual components

 United States Environmental Protection Agency

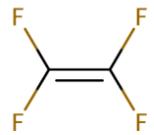
Home [Advanced Search](#) [Batch Search](#) [Lists](#) [Predictions](#) [Downloads](#) [Copy](#) [Share](#) [Submit Comment](#)

1-Hexene, 3,3,4,4,5,5,6,6,6-nonafluoro-, polymer with ethene and 1,1,2,2-tetrafluoroethene

68258-85-5 | DTXSID50880596
Searched by DSSTox Substance Id.

4 chemicals

Select all [Download](#) [Send to Batch Search](#) Relationship [CASRN](#) [DTXSID](#) [Mono.Mass](#) [Hide chemicals that are:](#) [Filter by Name or CASRN](#)

Searched Chemical	Monomer	Monomer	Monomer
<p>3 related chemical structures with this substance</p> <p>1-Hexene, 3,3,4,4,5,5,6,6,6-nonafluoro-, ... CASRN:68258-85-5 DTXSID:DTXSID50880596 Mono.Mass:0</p>	 <p>Tetrafluoroethylene CASRN:116-14-3 DTXSID:DTXSID6021325 Mono.Mass:99.993613</p>	<p>$H_2C=CH_2$</p> <p>Ethylene CASRN:74-85-1 DTXSID:DTXSID1026378 Mono.Mass:28.0313</p>	 <p>1H,1H,2H-Perfluoro-1-hexene CASRN:19430-93-4 DTXSID:DTXSID6047575 Mono.Mass:246.009104</p>

- DETAILS
- EXECUTIVE SUMMARY
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- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES**
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS



Discover.

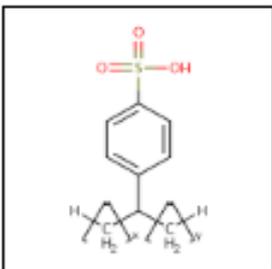
[About/Disclaimer](#)
[Accessibility](#)
[Privacy](#)

Connect.

[ACToR](#)
[DSSTox](#)
[Downloads](#)

Ask.

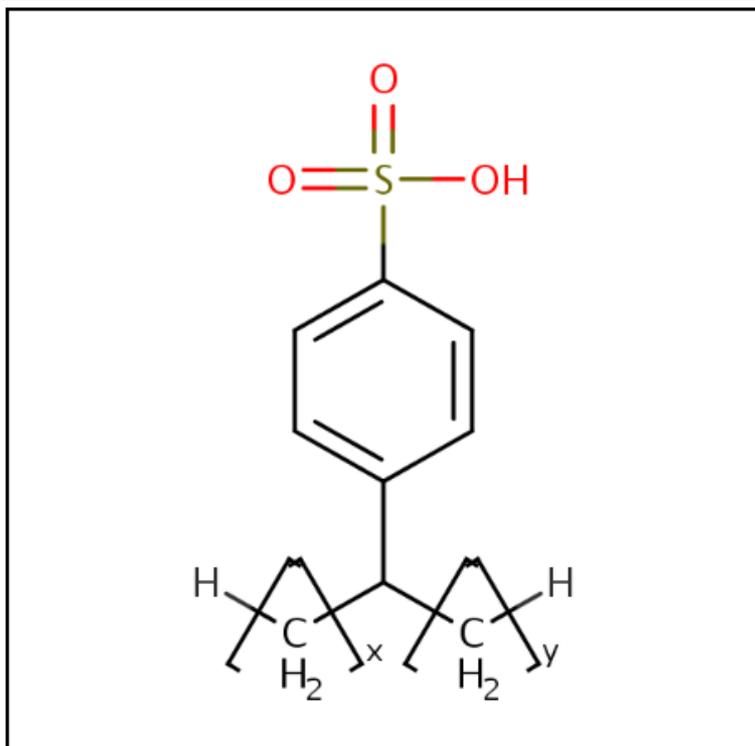
[Contact](#)
[Help](#)



Alkylbenzenesulfonate, linear

42615-29-2 | DTXSID3020041

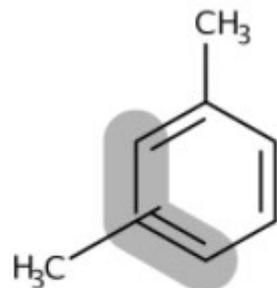
Searched by DSSTox Substance Id.



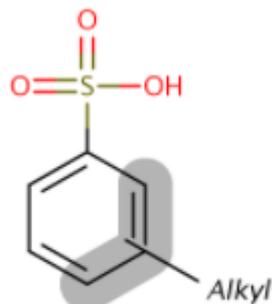
- Ambiguous representations of *some* structures are possible
- “Markush” representations can be valuable for describing and mapping chemicals

“Markush Structures”

https://en.wikipedia.org/wiki/Markush_structure



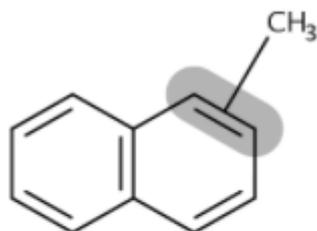
Xylenes
1330-20-7



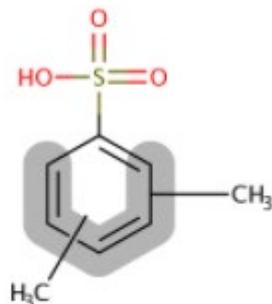
(C10-C16) Alkylbenzenesulfonic acid
68584-22-5



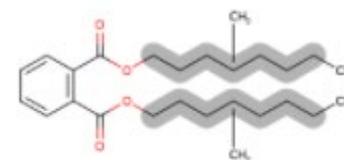
n-Nonylphenol
25154-52-3



Methyl-naphthalene
1321-94-4



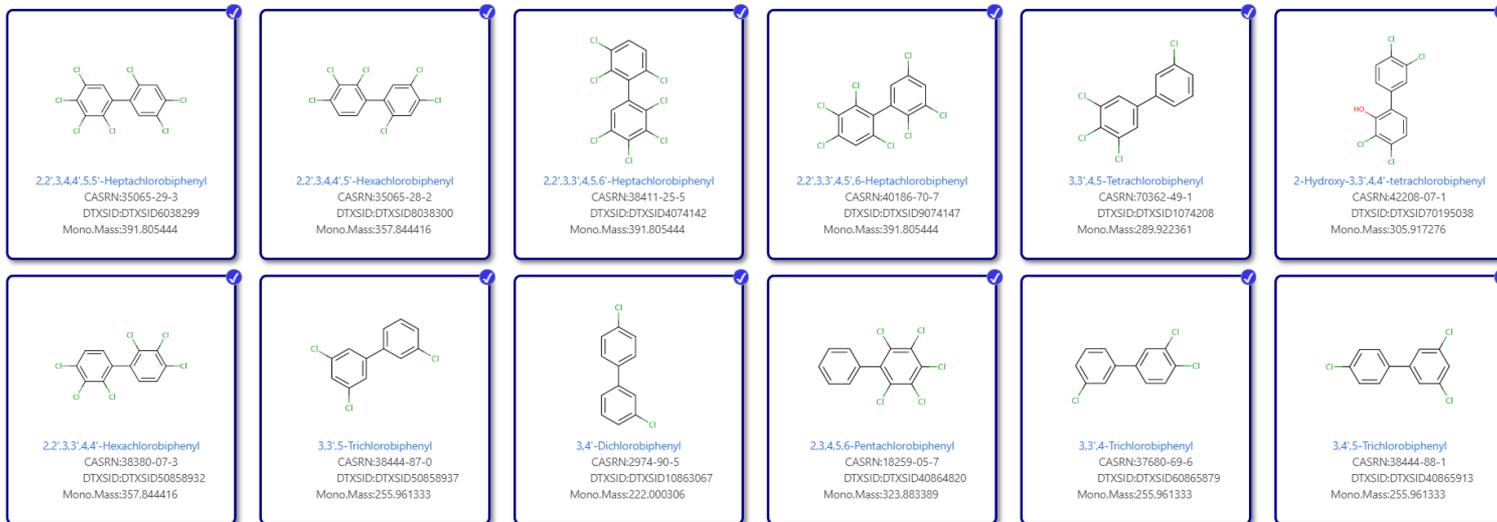
Sodium xylenesulfonate
1300-72-7



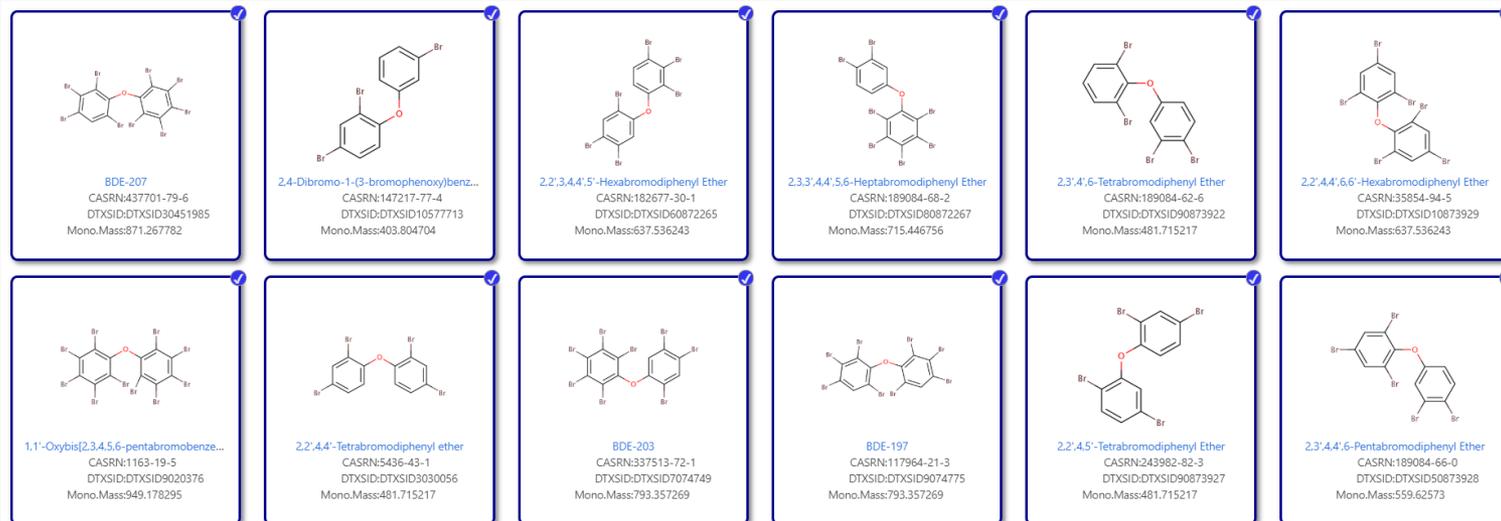
Diisononyl phthalate
28553-12-0

Chemical "grouping" – PCBs, PBDEs

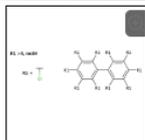
PCBs



PBDEs



Some Markush chemicals are bounded

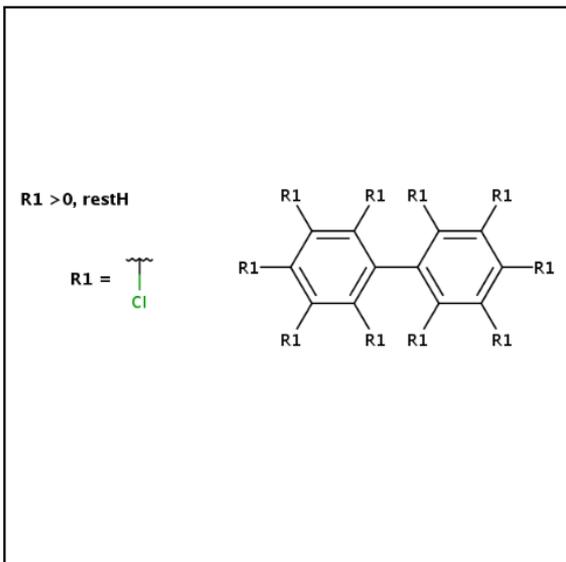


Polychlorinated biphenyls

1336-36-3 | DTXSID5024267

Searched by Expert Validated Synonym.

Previously 1-1 mapping



Successor Substances (209)

	CAS-RN	Relationship	Source
	32774-16-6	is a Representative Isomer of this	STN(DSSTox) ▼
	2051-60-7	is a Representative Isomer of this	Public ▼
	2051-61-8	is a Representative Isomer of this	Public ▼
	2051-62-9	is a Representative Isomer of this	Public ▼
	13029-08-8	is a Representative Isomer of this	Public ▼
	16605-91-7	is a Representative Isomer of this	Public ▼
	25569-80-6	is a Representative Isomer of this	Public ▼
	33284-50-3	is a Representative Isomer of this	Public ▼
	34883-43-7	is a Representative Isomer of this	Public ▼
	34883-39-1	is a Representative Isomer of this	Public ▼

Now Markush Enumeration

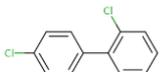
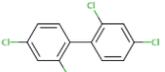
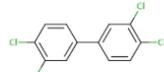
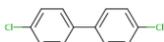
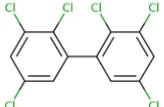
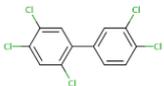
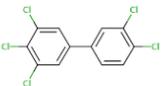
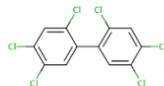
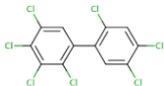
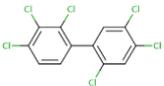
Polychlorinated biphenyls

1336-36-3 | DTXSID5024267

Searched by Expert Validated Synonym.

18 of 211 chemicals selected

Deselect all Download Send to Batch Search Relationship CASRN DTXSID Mono.Mass Unselected Filter by Name or CASRN

Markush Child	Markush Child	Markush Child	Markush Child	Markush Child
 <p>2,4'-Dichlorobiphenyl CASRN:34883-43-7 DTXSID:DTXSID0022511 Mono.Mass:222.000306</p>	 <p>2,2',4,4'-Tetrachlorobiphenyl CASRN:2437-79-8 DTXSID:DTXSID0022513 Mono.Mass:289.922361</p>	 <p>3,3',4,4'-Tetrachlorobiphenyl CASRN:32598-13-3 DTXSID:DTXSID0022514 Mono.Mass:289.922361</p>	 <p>4,4'-Dichlorobiphenyl CASRN:2050-68-2 DTXSID:DTXSID0022515 Mono.Mass:222.000306</p>	 <p>2,2':3,3':5,5'-Hexachlorobiphenyl CASRN:35694-04-3 DTXSID:DTXSID4030045 Mono.Mass:357.844416</p>
Markush Child	Markush Child	Markush Child	Markush Child	Markush Child
				

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

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LINKS

COMMENTS

UVCB: Complex Surfactants

DETAILS

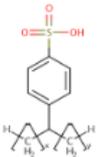
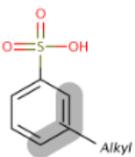
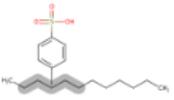
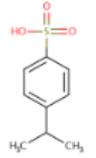
RELATED SUBSTANCES

PROPERTIES

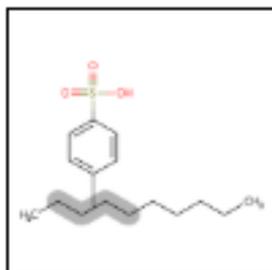
COMMENTS

25 chemicals

Select all Download Send to Batch Search Relationship DTXSID PubChem CPDAT Hide chemicals that are: Filter by Name or CASRI

<p>Searched Chemical</p>  <p>Alkylbenzenesulfonate, linear DTXSID: DTXSID3020041 PubChem: 0 CPDAT: 83</p>	<p>Component</p>  <p>(C10-C16) Alkylbenzenesulfonic acid DTXSID: DTXSID2028723 PubChem: 0 CPDAT: 132</p>	<p>Component</p> <p>2 related chemical structures with this substance</p> <p>Benzenesulfonic acid, C10-16-alkyl deriv... DTXSID: DTXSID7028724 PubChem: 0 CPDAT: 21</p>	<p>Component</p> <p>2 related chemical structures with this substance</p> <p>Benzenesulfonic acid, C10-13-alkyl deriv... DTXSID: DTXSID3029784 PubChem: 0 CPDAT: 179</p>	<p>Component</p> <p>4 related chemical structures with this substance</p> <p>Benzenesulfonic acid, dodecyl-, branche... DTXSID: DTXSID4049583 PubChem: 0 CPDAT: 22</p>
<p>Component</p> <p>1 related chemical structure with this substance</p> <p>Benzenesulfonic acid, C10-16-alkyl deriv... DTXSID: DTXSID7099894 PubChem: 0 CPDAT: 52</p>	<p>Component</p> <p>1 related chemical structure with this substance</p> <p>Benzenesulfonic acid, mono-C9-17-bran... DTXSID: DTXSID20100697 PubChem: 0 CPDAT: 16</p>	<p>Component</p>  <p>C12-linear alkyl benzene sulfonate DTXSID: DTXSID90891641 PubChem: 0 CPDAT: 0</p>	<p>Component</p>  <p>C10-linear alkylbenzenesulfonate DTXSID: DTXSID70891689 PubChem: 0 CPDAT: 0</p>	<p>Markush Child</p>  <p>4-Isopropylbenzenesulfonic acid DTXSID: DTXSID1044932 PubChem: 42 CPDAT: 0</p>

UVCB: Complex Surfactants

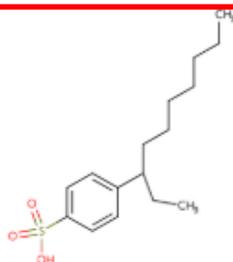


C10-linear alkylbenzenesulfonate

NOCAS_891689 | DTXSID70891689

Searched by DSSTox Substance Id.

Markush Child



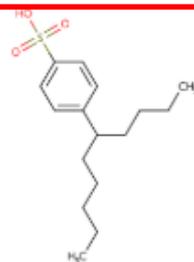
4-(Decan-3-yl)benzene-1-sulfonic acid

DTXSID: DTXSID20859618

PubChem: 0

CPDAT: 0

Markush Child



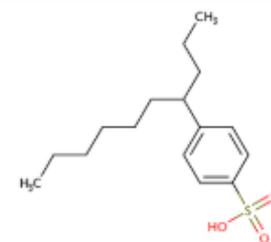
4-(decan-5-yl)benzene-1-sulfonic acid

DTXSID: DTXSID70881146

PubChem: 0

CPDAT: 0

Markush Child



4-(decan-4-yl)benzenesulfonic acid

DTXSID: DTXSID40891333

PubChem: 0

CPDAT: 0

Chemical Lists and Categories

EPAHFR: Hydraulic Fracturing

Home Advanced Search Batch Search Lists ▾ Predictions Downloads

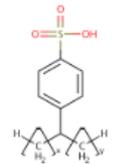
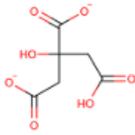
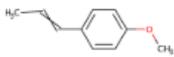
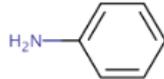
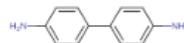
Lists of Chemicals 

List of Assays

WATER|EPA; Chemicals associated with hydraulic fracturing

Identifier substring search

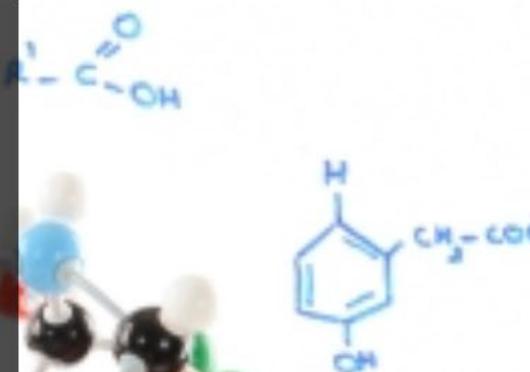
List

 <p>Alkylbenzenesulfonate, linear DTXSID: DTXSID3020041 PubChem: 0 CPDAT: 83</p>	<p>Cl NH₄</p> <p>Ammonium chloride DTXSID: DTXSID0020078 PubChem: 82 CPDAT: 260</p>	 <p>Diammonium citrate DTXSID: DTXSID5020079 PubChem: 19 CPDAT: 18</p>	<p>OH NH₄</p> <p>Ammonium hydroxide DTXSID: DTXSID4020080 PubChem: 83 CPDAT: 857</p>
 <p>Anethole DTXSID: DTXSID4020086 PubChem: 59 CPDAT: 33</p>	 <p>Aniline DTXSID: DTXSID8020090 PubChem: 284 CPDAT: 80</p>	 <p>Benzidine DTXSID: DTXSID2020137 PubChem: 112 CPDAT: 15</p>	 <p>Benzo(a)pyrene DTXSID: DTXSID2020139 PubChem: 161 CPDAT: 81</p>

TSCA Chemical Substance Inventory

CONTACT US

The Toxic Substances Control Act (TSCA) Chemical Substance Inventory contains all existing chemical substances manufactured, processed, or imported in the United States that do not qualify for an exemption or exclusion under TSCA. [This may be your starting place for interaction with EPA on TSCA regulatory matters.](#)



Nucleophiles (Nu):



O: H₂O, ROH, RCOO⁻
(Solvent: ...)



TSCA Inventory List

Active Non-confidential portion

EPA|TSCA: TSCA Inventory, active non-confidential portion

Search TSCAACTIVENONCONF Chemicals

Identifier substring search

List Details

11919 of 23514 chemicals visible

Select all

Download

Send to Batch Search

Default

↑

CASRN

DTXSID

Mono.Mass

No Structures

Filter by Name or CASRN

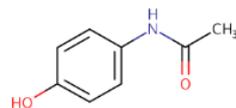


Acetamide

CASRN:60-35-5

DTXSID:DTXSID7020005

Mono.Mass:59.037114

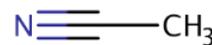


Acetaminophen

CASRN:103-90-2

DTXSID:DTXSID2020006

Mono.Mass:151.063329

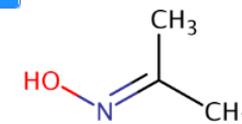


Acetonitrile

CASRN:75-05-8

DTXSID:DTXSID7020009

Mono.Mass:41.026549



Acetoxime

CASRN:127-06-0

DTXSID:DTXSID6020010

Mono.Mass:73.052764

Over 11,500 out of 23,500 have NO STRUCTURES

Batch Searching

- Singleton searches are useful but people generally want data on LOTS of chemicals!
- Typical questions
 - 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?
 - Can I include properties in the download file?

Batch Search Names

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

Step Five: Choose Data Fields to Download

Please enter one identifier per line

Select Input Type(s)

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

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

Buprenorphine
Codeine
Dextromethorphan
Dihydrocodeine
Dihydromorphine
Ethylmorphine
Fentanyl
Heroin
Hydrocodone
Hydromorphone

Display All Chemicals Download Chemical Data

**Excel
Download**

INPUT	FOUND_BY	DTXSID
Buprenorphine	Approved Name	DTXSID2022705
Codeine	Approved Name	DTXSID2020341
Dextromethorphan	Approved Name	DTXSID3022908
Dihydrocodeine	Approved Name	DTXSID5022936
Dihydromorphine	Approved Name	DTXSID7048908
Ethylmorphine	Approved Name	DTXSID1046760
Fentanyl	Approved Name	DTXSID9023049
Heroin	Synonym	DTXSID6046761
Hydrocodone	Approved Name	DTXSID8023131
Hydromorphone	Approved Name	DTXSID8023133
Ketamine	Approved Name	DTXSID8023187
Meperidine	Approved Name	DTXSID9023253
Methadone	Approved Name	DTXSID7023273
Morphine	Approved Name	DTXSID9023336

Add Other Data of Interest

Chemical Identifiers

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

Structures

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

Intrinsic And Predicted Properties

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

INPUT	DTXSID	CASRN	MOLECULAR_FORMULA	MONOISOTOPIC MASS	MS_READY_SMILES
Buprenorph	DTXSID202	52485-79-7	C29H41NO4	467.3035588	[H]C12CC3=C4C
Codeine	DTXSID202	76-57-3	C18H21NO3	299.1521435	[H]C12CC3=C4C
Dextrometh	DTXSID302	125-71-3	C18H25NO	271.1936144	[H]C12CC3=C(C=
Dihydrocod	DTXSID502	125-28-0	C18H23NO3	301.1677936	[H]C12CC3=C4C
Dihydromor	DTXSID704	509-60-4	C17H21NO3	287.1521435	[H]C12CC3=C4C
Ethylmorph	DTXSID104	76-58-4	C19H23NO3	313.1677936	[H]C12CC3=C4C
Fentanyl	DTXSID902	437-38-7	C22H28N2O	336.2201635	CCC(=O)N(C1CC
Heroin	DTXSID604	561-27-3	C21H23NO5	369.1576228	[H]C12CC3=C4C
Hydrocodor	DTXSID802	125-29-1	C18H21NO3	299.1521435	[H]C12CC3=C4C
Hydromorph	DTXSID802	466-99-9	C17H19NO3	285.1364935	[H]C12CC3=C4C
Ketamine	DTXSID802	6740-88-1	C13H16ClNO	237.0920418	CNC1(CCCCC1=
Meperidine	DTXSID902	57-42-1	C15H21NO2	247.1572289	CCOC(=O)C1(CC
Methadone	DTXSID702	76-99-3	C21H27NO	309.2092645	CCC(=O)C(CC(C)
Morphine	DTXSID902	57-27-2	C17H19NO3	285.1364935	[H]C12CC3=C4C
Morphinone	DTXSID501	467-02-7	C17H17NO3	283.1208434	[H]C12CC3=C4C
Naloxone	DTXSID802	465-65-6	C19H21NO4	327.1470582	[H]C12CC3=C4C
Naltriben	-	-	-	-	-
Oxycodone	DTXSID502	76-42-6	C18H21NO4	315.1470582	[H]C12CC3=C4C
Oxymorpho	DTXSID502	76-41-5	C17H19NO4	301.1314081	[H]C12CC3=C4C
Propoxyph	DTXSID102	469-62-5	C22H29NO2	339.2198292	CCC(=O)OC(CC1
Sufentanil	DTXSID602	56030-54-7	C22H30N2O2S	386.2027994	CCC(=O)N(C1=C
Tramadol	DTXSID908	27203-92-5	C16H25NO2	263.188529	COC1=CC=CC(=

Related Substance Relationships

Enhanced Data Sheets

- MetFrag Input File (Beta)
- ToxPrint single fingerprints
- Abstract Sifter Input File (Beta)
- Synonyms and Identifiers
- Related Substance relationships
- ToxPrint fingerprints (ChemoTyper f
- Associated ToxCast Assays

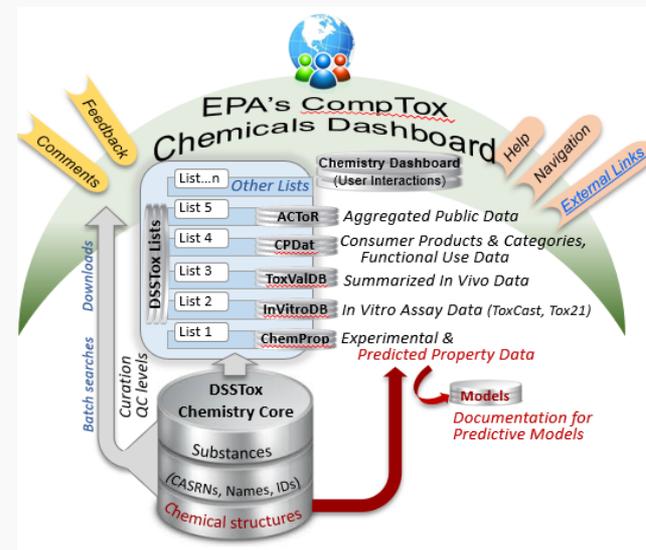
- EPA: National-Scale Air
- EPA: PPRTV Chemical R
- EPA: Provisional Adviso
- EPA: Safer Choice Chem

Selecting this checkbox provides a separate Excel worksheet containing the relationship between two chemicals. The output file includes the DTXSIDs and names/CASRN between the input list and the related chemical. Relationships include, for example, polymer, components, salt form, transformation product and other relationships.

	A	B	C	D	E	
1	INPUT	DTXSID	PREFERRED_NAME	HAS_RELATIONSHIP_WITH	RELATED_DTXSID	RELATED_PREFERRED_NAME
2	xylenes	DTXSID2021446	Xylenes	Transformation Product	DTXSID40176394	N-Benzoylalanine
3	xylenes	DTXSID2021446	Xylenes	Component	DTXSID6026298	m-Xylene
4	xylenes	DTXSID2021446	Xylenes	Component	DTXSID3021807	o-Xylene
5	xylenes	DTXSID2021446	Xylenes	Component	DTXSID2021868	p-Xylene
6	xylenes	DTXSID2021446	Xylenes	Predecessor: Component	DTXSID9021421	Xylenes; defined mixture 1
7	xylenes	DTXSID2021446	Xylenes	Predecessor: Component	DTXSID7021447	Xylenes; defined mixture 2
8	xylenes	DTXSID2021446	Xylenes	Predecessor: Component	DTXSID30891529	Total Petroleum Hydrocarbons
9	xylenes	DTXSID2021446	Xylenes	Markush Child	DTXSID3021807	o-Xylene
10	xylenes	DTXSID2021446	Xylenes	Markush Child	DTXSID6026298	m-Xylene
11	xylenes	DTXSID2021446	Xylenes	Markush Child	DTXSID2021868	p-Xylene

Conclusion

- Building an integrated hub for environmental chemistry data to serve computational toxicology
- Transparent access to data and models – file downloads, SQL data dumps and web services
- Expansion of functionality to serve all data streams generated by NCCT across the agency & community
- Data **QUALITY** is a key focus - ongoing curation
- Ongoing API development will provide enhanced access to data streams





Credit: the Research Triangle Foundation

EPA-RTP

- *An enormous team of contributors from CCTE, especially the IT software development team*
- *Our curation team for their care and focus on data quality*
- *Multiple centers and laboratories across the EPA*
- *Many public domain databases and open data contributors*

Antony Williams

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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**

 CrossMark

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>