



Physicians
Committee
for Responsible Medicine



Introduction to the US EPA CompTox Chemicals Dashboard

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October 23rd 2020

- **A publicly accessible website** delivering access:
 - ~882,000 chemicals with related property data
 - Experimental and predicted physicochemical property data
 - Experimental Human and Ecological hazard data
 - Integration to “biological assay data” for 1000s of chemicals
 - Information regarding consumer products containing chemicals
 - Links to other agency websites and public data resources
 - “Literature” searches for chemicals using public resources
 - “Batch searching” for thousands of chemicals

CompTox Chemicals Dashboard

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



EPA United States Environmental Protection Agency

875 Thousand Chemicals

SEARCH

Chemicals Product/Use Categories Assay/Gene

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey

Identifier substring search

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

EPA United States Environmental Protection Agency

Batch Search BATCH SEARCH

Step Four: Select Data Output Format and Choose Data Fields to Download

Please enter one identifier per line

Select Input Type(s)

- Identifiers
- Chemical Name
- CASRN
- InChIKey
- DQ/Tox Substance ID
- BSL/Chem Compound ID
- InChIKey Synonym
- MS-Ready Formula
- Exact Formula
- Molecular Weight

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

107-22-2
86-29-7
14024-55-6
33484-55-5
7784-40-9
1933-46-9
86232-26-5
2122-70-5
72833-17-6
7786-81-4

Select Output Format: Excel

Download Chemical Data

Customize Results

- Select All
- Select All in Lists
- Chemical Identifiers
 - DTXSID
 - Chemical Name

Presence in Lists:

- Pharmaceuticals from ZINC15
- Accession External/In-house Substances List and Threshold Planning Quantities
- ASLCA Acute Exposure Guideline Levels
- Arthropods Metals
- Androgen/Androgen Receptor Chemicals

EPA United States Environmental Protection Agency

Latest News

Read more news

List of Terpenes added to Dashboard

19th, 2019 at 12:28:28 AM

Chemical list related to terpenes found in vape has been added to the dashboard and is available at: comptox.epa.gov/dashboard/chemical_lists/VAPETERPENES

EPA United States Environmental Protection Agency

TOX DATA

Bisphenol A
80-05-7 | DTXSID7020182
Searched by Expert Validated Synonym.

Hazard

Human

Details: EXECUTIVE SUMMARY, PROPERTIES, ENV. FATE/TRANSPORT, HAZARD, ADME, EXPOSURE, BIOACTIVITY, SIMILAR COMPOUNDS, GENRA (BETA), RELATED SUBSTANCES, SYNONYMS, LITERATURE, LINKS

TOXCAST SUMMARY

ESFP21
TOXCAST70021
PUBCHEM

EPA United States Environmental Protection Agency

ACROSS

Find articles quickly, with links to full abstracts

Input	Abstract	Full	PMID	Year	Title	Authors	Journal	Relevance
2	3	2	18	2014	Developmental treatment with ethoxyestradiol, but not bisphenol A, causes alterations in sex...	Pargison, Lar, Kising	Toxicological sciences: an official journal of the So...	100%
2	3	2	18	2015	Impact of Low-Dose Oral Exposure to Bisphenol A (BPA) on Juvenile and Adult Rat Endocrine...	Riebel, Genevieve; Adams, Rick; Ayler, Michael	Toxicological sciences: an official journal of the So...	100%
2	2	2	18	2014	Investigation of the effects of subchronic low-dose oral exposure to bisphenol A (BPA) and eth...	Riebel, Genevieve; Adams, Rick; Ayler, Michael; Levis, Van...	Toxicological sciences: an official journal of the So...	100%
2	2	2	18	2014	Toxicity evaluation of bisphenol A administered to geriatric Sprague-Dawley rats from postna...	Dickson, Camacho; Lewis, Vandenberg; Leland...	Toxicological sciences: an official journal of the So...	100%
2	2	2	18	2012	Endocrine disruptive effects of dietary exposure to bisphenol A in the juvenile endocrine o...	Kang, Seung; Chinn, Quyen; Choi, Dong-Hyup	International journal of toxicology	100%
2	2	2	18	2007	Endocrine activity of chemicals detected in sewage treatment plant effluents as determined...	Kasuya, Masahiko; Saito, Kazuo; Shimizu, Shiro; Hagi...	Environmental toxicology and chemistry	100%
2	1	1	1	2018	In vitro-in vivo extrapolation (IVIVE) in PBTK modeling for animal-free risk assessment app...	Fabian, Connor; Erik, Wilbert; Hernandez, Heide...	Archives of toxicology	100%
2	1	0	1	2017	Phthalate bisphenol A (BPA) exposure alters the transcription of the neonatal rat organolep...	Alvarado, Ana; Palacios	Neurotoxicology	100%
2	1	0	1	2017	Effect of prenatal bisphenol A exposure on the volume of sexually dimorphic nuclei of prena...	Alvarado, Ana; Choi, Prasad	Neurotoxicology	100%
2	1	1	1	2016	Impact of Low-Dose Oral Exposure to Bisphenol A (BPA) on the Neonatal Rat Hypothalamus...	Alvarado, Ana; Choi, Prasad	Endocrinology	100%
2	1	1	1	2016	Comparison of Electrochemical Immunosensors and Advantages for Detection of Small Orga...	Phu, Shi; Reisinger, Nicole; Anagnost...	Biosensors	100%
2	1	1	1	2016	Neurotoxicology and behavioral effects of maternal exposure to bisphenol A in female mice...	Stank, Pook; Gupta, Parvinder; Gupta-Prasad, K...	The Journal of endocrinology	100%
2	1	1	1	2016	Endocrine activity of chemicals detected in sewage treatment plant effluents as determined...	Kasuya, Masahiko; Saito, Kazuo; Shimizu, Shiro; Hagi...	Neurotoxicology	100%
2	1	1	1	2010	Neonatal exposure to bisphenol A and reproductive and endocrine alterations resembling the...	Fernandez, Bourgeois; Liu-Lattin, Libertan	Environmental health perspectives	100%
2	1	0	1	2006	Two-generation reproductive toxicity study of dietary bisphenol A in CD-1 (B6) mice.	Tal, Myra; Mar, Susan; Castillo, Vanessa; Sway, D...	Toxicological sciences: an official journal of the So...	100%

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BIOACTIVITY

Bisphenol A
80-05-7 | DTXSID7020182
Searched by Expert Validated Synonym.

Chemical Activity Summary

TOXCAST DATA

ASSAY DETAILS

ACSD 0481 1717
Scaled Top: 0.10
Assay Endpoint Name: OT_EF_EF02a_0481
Assay Description: 742
Gene Symbol: ESR1
Organism Name: Human
Tissue: Kidney
Assay Format Type: cell based
Biological Process Target: protein stabilization
Analysis Direction: positive
Intended Target Family: nuclear receptor
Description: Data from the assay component OT_EF_EF02a_0481 was analyzed into a 1 assay endpoint. This assay endpoint, OT_EF_EF02a_0481, was analyzed in the positive fitting direction relative to DMG0 as the negative control and baseline of activity. Using a type of binding register, measure of receptor for gene-signal activation can be used to understand the binding in the pathway level as they relate to the gene ESR1. Furthermore, this assay endpoint can be extended to a primary market because the performed assay has only produced 1 assay endpoint. To generalize the intended target to other related targets, this assay endpoint is associated to the "nuclear receptor" implied target family where the similarity is "similar".

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SIMILARITY

Bisphenol A
80-05-7 | DTXSID7020182
Searched by Expert Validated Synonym.

Searched with a similarity threshold of 0.8

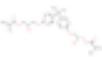
778 of 798 chemicals visible

Select All Download Send to Batch Search Similarity 0.8

Similar Compounds:

- 4-Cumylphenol
CASRN:699-84-4
DTXSID:DTXSID0202556
TOXCAST:307779
- 4-(1,1-diphenylethyl)phenol
CASRN:6938-97-2
DTXSID:DTXSID0528558
TOXCAST:1
- 4-(1-Phenylethyl)phenol
CASRN:1571-73-1
DTXSID:DTXSID0505144
TOXCAST:76275
- 4,4'-Diphenyl-1,1'-oxybisphenol
CASRN:2765-84-8
DTXSID:DTXSID0207712
TOXCAST:340479
- 4-Triphenylethylphenol
CASRN:678-86-9
DTXSID:DTXSID0075172
TOXCAST:1

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

- Three searches from the home page
 - Chemicals (Names, CASRN, Substring)
 - Product/Use Categories (Kristin...)
 - Assay Gene (Katie...)
- Searching millions of synonyms and includes Active, Deleted and Alternate CASRNs

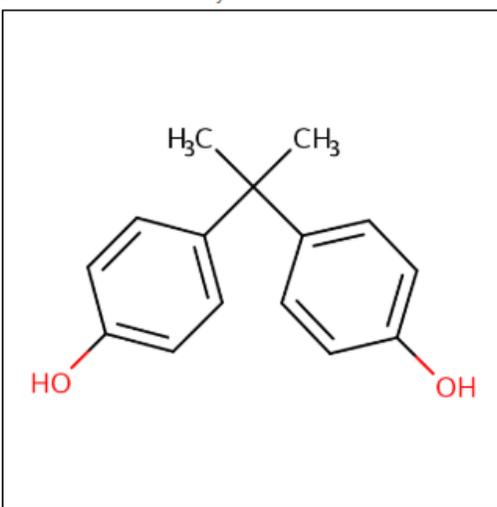
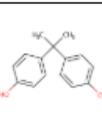
 United States Environmental Protection Agency

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

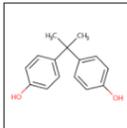
Linked Substances

Presence in Lists

Record Information

Quality Control Notes

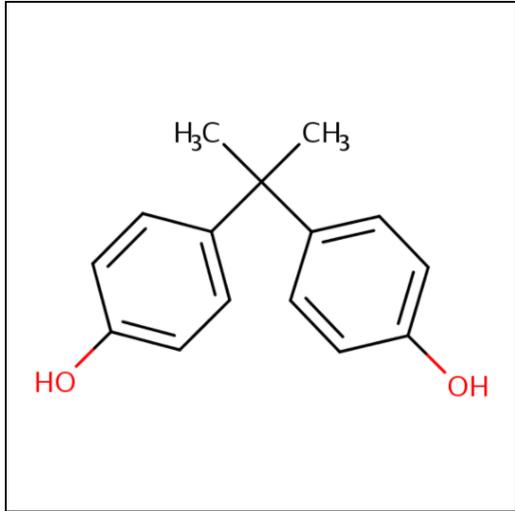
Linked Substances: Mixtures and Components, Similar Compounds



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.



Wikipedia

Quality Control Notes

Intrinsic Properties

Structural Identifiers

Linked Substances

Same Connectivity: 6 records (based on first layer of InChI)

Mixtures, Components and Isotopomers: DTXCID30182: 27 records;

Similar Compounds: 430 records (based on Tanimoto coefficient >0.8)

Presence in Lists

MS-Ready Mappings of Bisphenol A (Isotopes pre-filtered)

22 of 27 chemicals visible

Select all Download Send to Batch Search Default 0 DTXSID X CASRN X TOXCAST X

Isotopes X Filter by Name or CASRN

<p>Bisphenol A DTXSID:DTXSID7020182 CASRN:80-05-7 TOXCAST:217/1152</p>	<p>Disodium 4,4'-isopropylidenediphenolate DTXSID:DTXSID0027480 CASRN:2444-90-8 TOXCAST:-</p>	<p>Barium(2+) 4,4'-isopropylidenediphenolate DTXSID:DTXSID90240211 CASRN:94006-29-8 TOXCAST:-</p>	<p>PUBCHEM_24208743 DTXSID:DTXSID60639875 CASRN:62611-29-4 TOXCAST:-</p>	<p>4,4'-(Propane-2,2-diyldiphenol)-1,2-diol DTXSID:DTXSID10724048 CASRN:53965-19-8 TOXCAST:-</p>	<p>Phosphoric acid-4,4'-(propane-2,2-diyldiphenol) DTXSID:DTXSID10741891 CASRN:4235-90-9 TOXCAST:-</p>
<p>Methanesulfonic acid-4,4'-(propane-2,2-diyldiphenol) DTXSID:DTXSID10767819 CASRN:129236-44-8 TOXCAST:-</p>	<p>Carbamic acid-4,4'-(propane-2,2-diyldiphenol) DTXSID:DTXSID60776870 CASRN:15498-23-4 TOXCAST:-</p>	<p>Carbonic acid-4,4'-(propane-2,2-diyldiphenol) DTXSID:DTXSID50855401 CASRN:34074-60-7 TOXCAST:-</p>	<p>Phenol 4,4'-(1-methylethylidene)bis-2-phenol DTXSID:DTXSID20888786 CASRN:99904-21-9 TOXCAST:-</p>	<p>4,4'-(Propane-2,2-diyldiphenol)-2,2'-diol DTXSID:DTXSID40911742 CASRN:110553-33-8 TOXCAST:-</p>	<p>Carbononitric chloride-4,4'-(propane-2,2-diyldiphenol) DTXSID:DTXSID60915606 CASRN:84350-18-2 TOXCAST:-</p>

Searched with a similarity threshold of 0.8

418 of 430 chemicals visible

Select all Download Send to Batch Search Similarity 0 DTXSID X CASRN X TOXCAST X Similarity X

Isotopes X Filter by Name or CASRN

<p>4-Cumylphenol DTXSID:DTXSID3022536 CASRN:599-64-4 TOXCAST:313/943 Similarity:1.00</p>	<p>4-(1,1-diphenylethyl)phenol DTXSID:DTXSID50288558 CASRN:6938-97-2 TOXCAST:- Similarity:1.00</p>	<p>4,4'-(1-Phenylethylidene)bisphenol DTXSID:DTXSID5051444 CASRN:1571-75-1 TOXCAST:79/273 Similarity:1.00</p>	<p>4,4',4''-Ethane-1,1,1-triyltriphenol DTXSID:DTXSID2037712 CASRN:27955-94-8 TOXCAST:321/871 Similarity:1.00</p>	<p>4-(Triphenylmethyl)phenol DTXSID:DTXSID8075172 CASRN:978-86-9 TOXCAST:- Similarity:1.00</p>
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Presence in Lists

Presence in Lists

Federal

- EPA Regional Screening Levels Data Chemicals List
- EPA: Underground Storage Tanks (USTs)
- EPA: IRIS Chemicals
- TOXCASST_PhaseII - EPA ToxCast Screening Library (Phase II Subset)
- TOXCASST_PhaseIII - EPA ToxCast Screening Library (Phase II Subset)
- TOXCASST_Ph2 - EPA ToxCast Screening Library (ph2 Subset)
- CHEMINV: EPA Chemical Inventory for ToxCast
- TOXCASST: EPA ToxCast Screening Library
- ENDOCRINE: EDSP Universe of Chemicals
- ECOTOX: Ecotoxicology knowledgebase
- WATER|EPA: Chemicals in hydraulic fracturing fluids Table H-2
- WATER|EPA: Chemicals associated with hydraulic fracturing
- NIOSH: International Chemical Safety Cards
- MASSPECDB: National Environmental Methods Index
- EPA: Chemicals mapped to HERO
- EPA: PPRTV Chemical Report
- EPA: Consumer Products Suspect Screening Result
- TOXCASST: EPA ToxCast Screening Assay In Vitro DB Version 3
- EPA: High Production Volume List
- CHEMINV: ToxCast/Tox21 Chemical inventory available as DMSO solutions (20181123)
- TOX21SL: Tox21 Screening Library
- LIST: Substances Added to Food (formerly EAFUS)
- TSCA Active Inventory non-confidential portion (updated March 20th 2020).

US State

None.

International

- Canadian Domestic Substances List 2019
- FOOD: EFSA OpenFoodTox
- NORMAN: KEMI List of Substances on the Market

- ~882,000 chemicals are associated with > 280 lists
- Lists are segregated into
 - Federal
 - US State
 - International
 - Other
- Chemicals can be present in multiple lists – with clickthrough

Lists of Lists of Chemicals

>280 lists and growing

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

Lists of Chemicals
List of Assays

Select List

Download Columns 10 Search query Copy page URL

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
40CFR1164	40CFR116.4 Designation of Hazardous Substances (Above Ground Storage Tanks)	2020-06-25	331	Hazardous Substance List (40CFR116.4): related to Above Ground Storage Tanks
40CFR355	40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities	2018-01-05	354	Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378)
ACSREAG	LIST: ACS Reagent Chemicals	2017-04-14	405	The ACS Committee on Analytical Reagents sets purity specifications for almost 500 reagent chemicals and over 500 standard-grade reference materials.
AEGLVALUES	AEGLS: 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	LIST: Algal Toxins	2018-05-04	55	A list of Algal Toxins of potential interest
AMINOACIDS	CATEGORY: Amino acids	2019-02-04	20	Amino acids are organic compounds containing amine (-NH2) and carboxyl (-COOH) functional groups, along with a side chain (R group) specific to each amino acid.
AMPHIBOLES	LIST: Amphiboles	2019-03-26	23	Amphiboles are an important group of inosilicate minerals.
ANTIBIOTICS	CATEGORY PHARMACEUTICALS: Antibiotics	2019-11-16	170	List of antibiotics and related compounds
ANTIMICROBIALS	CATEGORY WIKILIST ANTIMICROBIALS: List of Antimicrobials from Wikipedia	2020-10-11	289	A list of antimicrobials extracted from Wikipedia.
AOPSTRESSORS	List of Adverse Outcome Pathway Stressors	2020-06-05	349	List of Adverse Outcome Pathway Stressors from the AOP Database

First << < 1 2 3 4 5 6 7 8 9 10 > >> Last

Showing 1 to 10 of 281 records

List of Chemicals

Example: Acute Exposure Guideline Levels

- Chemical List Examples
 - Disinfection by-products
 - EPA Pesticide Search DB
 - Consumer Products DB
 - Chemicals in Biosolids
 - ATSDR Toxicological Profiles
 - Canadian Domestic Substances
 - Chemical Inventory for ToxCast
 - EFSA OpenFoodTox
 - EDSP Universe of Chemicals
 - Hydraulic Fracturing Chemicals

AEGLS: Acute Exposure Guideline Levels

Search AEGLVALUES Chemicals
 Identifier substring search

List Details

Description: Acute Exposure Guideline Level (AEGLs) values are intended to protect most individuals in the general population, including those that might be particularly susceptible to the harmful effects of the chemicals. Acute exposure guideline levels (AEGLs) describe the human health effects from once-in-a-lifetime, or rare, exposure to airborne chemicals. Used by emergency responders when dealing with chemical spills or other catastrophic exposures, AEGLs are set through a collaborative effort of the public and private sectors worldwide.

Number of Chemicals: 174

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

174 chemicals

Excel
TSV
SDF

CC#N
Acetonitrile
DTXSID:DTXSID7020009
CASRN:75-05-8
TOXCAST:0/235

C=CC=O
Acrolein
DTXSID:DTXSID5020023
CASRN:107-02-8
TOXCAST:2/235

C=CC#N
Acrylonitrile
DTXSID:DTXSID5020029
CASRN:107-13-1
TOXCAST:10/434

C=CCO
Allyl alcohol
DTXSID:DTXSID8020044
CASRN:107-18-6
TOXCAST:17/426

- Five full time curators register and curate data to elevate quality

Record Information

 **Citation:** U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. <https://comptox.epa.gov/dashboard/DTXSID0020022> (accessed October 18, 2020), 5-(2-Chloro-4-(trifluoromethyl)phenoxy)-2-nitrobenzoic acid

Data Quality:

- Level 1: Expert curated, highest confidence in accuracy and consistency of unique chemical identifiers
- Level 2: Expert curated, unique chemical identifiers using multiple sources**
- Level 3: Programmatically curated from high quality EPA source, unique chemical identifiers
- Level 4: Programmatically curated from ChemID, unique chemical identifiers have been manually reviewed
- Level 5: Programmatically curated from ACToR or PubChem, unique chemical identifiers

Computational Toxicology 12 (2019) 100096

Contents lists available at [ScienceDirect](#)



Computational Toxicology

journal homepage: www.elsevier.com/locate/comtox



EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research

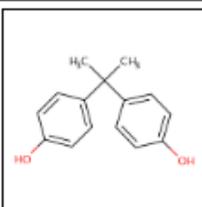
Christopher M. Grulke^a, Antony J. Williams^a, Inthirany Thillanadarajah^b, Ann M. Richard^{a,*}

^a National Center for Computational Toxicology, Office of Research & Development, US Environmental Protection Agency, Mail Drop D143-02, Research Triangle Park, NC 27711, USA

^b Senior Environmental Employment Program, US Environmental Protection Agency, Research Triangle Park, NC 27711, USA



Properties, Fate and Transport



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

Property

Summary

Summary

Download

Columns

Property	Experimental average	Predicted average	Experimental median	Predicted median
LogKow: Octanol-Water	3.32 (1)	3.30		3.39
Melting Point	155 (7)	140	156	144
Boiling Point	200 (1)	360		355
Water Solubility	8.55e-4 (3)	8.78e-4	5.26e-4	7.56e-4
Vapor Pressure	-	6.83e-7		1.51e-7
Flash Point	-	190		190
Surface Tension	-	46.0		
Index of Refraction	-	1.60		
Molar Refractivity	-	68.2		

Properties, Fate and Transport

e.g. Solubility

 Download Experimental Data ▼

Source	Result
PhysPropNCCT	5.26e-4
Tetko et al. J. Chem. Inf. and Comp. Sci. 41.6 (2001): 1488-1493	1.51e-3
Kovdienko, et. al. Molecular informatics 29.5 (2010): 394-406.	5.25e-4

Source	Result	Calculation Details
EPISUITE	7.56e-4	Not Available
NICEATM	1.31e-3	Not Available
TEST	1.24e-3	TEST Report
OPERA	5.44e-4	OPERA Model Report [Inside AD]
OPERA2	5.35e-4	Not Available



Journal
SAR and QSAR in Environmental Research >
Volume 27, 2016 - Issue 11: 17th International Conference on QSAR in Environmental and Health Sciences (QSAR 2016) - Part II. Guest Editors: C.G. Barber and G.J. Myatt

1,711

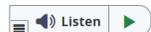
Views

47

CrossRef citations
to date

21

Altmetric



Articles

An automated curation process for addressing chemical errors and inconsistencies in public domain QSAR modelling^{\$}

K. Mansouri, C. M. Grulke, A. M. Richard, R. S. Judson & A. J. Williams
Pages 911-937 | Received 03 Sep 2016, Accepted 24 Oct 2016, Published online 12 Nov 2016

Download citation | <https://doi.org/10.1080/1062936X.2016.1222222>

Journal of Cheminformatics

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Research article | [Open Access](#) | Published: 08 March 2018

OPERA models for predicting physicochemical properties and environmental fate of chemicals

[Kamel Mansouri](#) , [Chris M. Grulke](#), [Richard S. Judson](#) & [Antony J. Williams](#)

Journal of Cheminformatics **10**, Article number: 10 (2018) | [Cite this article](#)

6598 Accesses | 49 Citations | 25 Altmetric | [Metrics](#)

Journal of Cheminformatics

Home About Articles Submission Guidelines About The Editors Calls For Papers

Research article | [Open Access](#) | Published: 18 September 2019

Open-source QSAR models for pKa prediction using multiple machine learning approaches

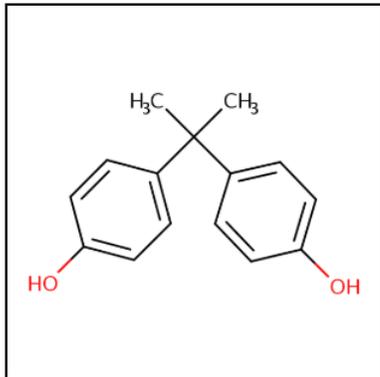
[Kamel Mansouri](#) , [Neal F. Cariello](#), [Alexandru Korotcov](#), [Valery Tkachenko](#), [Chris M. Grulke](#), [Catherine S. Sprankle](#), [David Allen](#), [Warren M. Casey](#), [Nicole C. Kleinstreuer](#) & [Antony J. Williams](#)

Journal of Cheminformatics **11**, Article number: 60 (2019) | [Cite this article](#)

9334 Accesses | 8 Citations | 20 Altmetric | [Metrics](#)

Properties, Fate and Transport

e.g. logP



Model Results

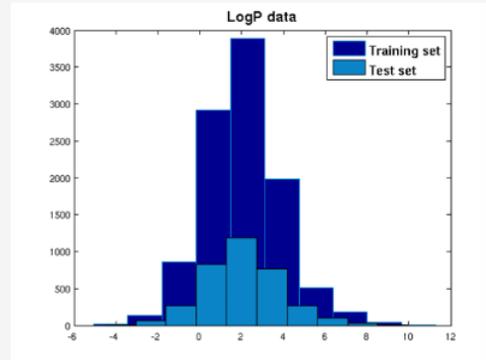
Predicted value: 3.35

Global applicability domain: Inside

Local applicability domain index: 0.877

Confidence level: 0.748

Model Performance

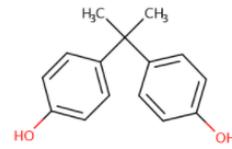


QMRF

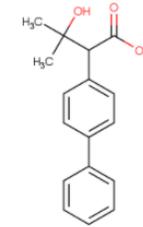
5-fold CV (75%)	
Q2	RMSE
0.850	0.690

od.epa.gov/dashboard/advanced_search/index

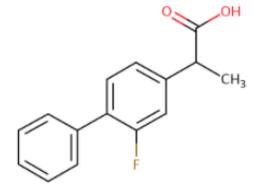
Nearest Neighbors from the Training Set



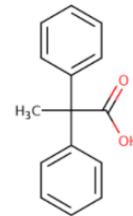
Bisphenol A
Measured: 3.32
Predicted: 3.32



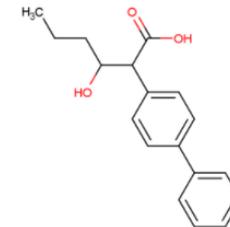
BUTANOIC ACID, 2-(4-BIPHENYL)-3-HYDROXY-3-METHYL
Measured: 3.25
Predicted: 3.25



Flurbiprofen
Measured: 4.16
Predicted: 4.16



2,2-Diphenylpropionic acid
Measured: 2.69
Predicted: 2.69



3-OH-2-(4-BIPHENYL)HEXANOIC ACID
Measured: 3.75
Predicted: 3.75

Predictions for New Chemicals

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

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

Search

Atrazine

Atrazine mercapturate

Atrazine mixture with butylate

Select properties to predict

T.E.S.T.

- Toxicological properties
 - 96 hour fathead minnow LC50
 - 48 hour D. magna LC50
 - 48 hour T. pyriformis IGC50
 - Oral rat LD50
 - Bioconcentration factor
 - Developmental toxicity
 - Ames mutagenicity
 - Estrogen Receptor RBA
 - Estrogen Receptor Binding
- Physical properties
 - Normal boiling point
 - Melting point
 - Flash point
 - Vapor pressure
 - Density
 - Surface tension
 - Thermal conductivity
 - Viscosity
 - Water solubility

P

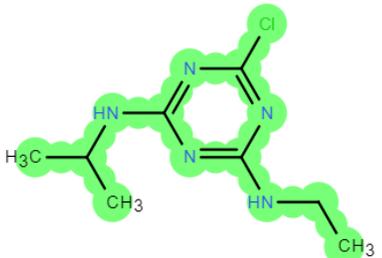
F

Cl

Br

I

PT



Chiral

Calculate

Predictions for New Chemicals

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

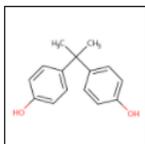


Provider: T.E.S.T.

 Download Summary 

Property	Experimental Value	Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50		3.969 -Log10(mol/L) 22.469 mg/L	3.936 -Log10(mol/L) 24.234 mg/L	3.742 -Log10(mol/L) 37.882 mg/L	4.135 -Log10(mol/L) 15.355 mg/L	4.064 -Log10(mol/L) 18.079 mg/L
48 hour D. magna LC50		3.791 -Log10(mol/L) 33.887 mg/L	3.568 -Log10(mol/L) 56.592 mg/L	4.243 -Log10(mol/L) 11.976 mg/L	3.832 -Log10(mol/L) 30.824 mg/L	3.521 -Log10(mol/L) 63.123 mg/L
48 hour T. pyriformis IGC50			2.986 -Log10(mol/L) 216.359 mg/L			
Oral rat LD50		2.439 -Log10(mol/kg) 761.182 mg/kg	2.355 -Log10(mol/kg) 924.254 mg/kg			2.524 -Log10(mol/kg) 626.882 mg/kg
Bioconcentration factor		0.847 Log10 7.038	0.906 Log10 8.051	0.690 Log10 4.903	0.820 Log10 6.607	0.974 Log10 9.409
Developmental toxicity		true	true	true		
Ames mutagenicity		false	true			false
Estrogen Receptor RBA						
Estrogen Receptor Binding		false	false	false	false	
Normal boiling point		315.9 °C	318.0 °C		345.4 °C	284.3 °C
Melting point		114.0 °C	105.0 °C		79.4 °C	157.7 °C
Flash point		176.1 °C	180.1 °C		172.5 °C	175.7 °C
Vapor pressure		-6.072 Log10(mmHg) 8.464*10^-7 mmHg	-6.164 Log10(mmHg) 6.851*10^-7 mmHg		-5.679 Log10(mmHg) 2.093*10^-6 mmHg	-6.374 Log10(mmHg) 4.23*10^-7 mmHg

Hazard Data (Human and Eco)



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.

DETAILS

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PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

SAFETY

GHS DATA

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

DataType

Point of Departure

Download

More

Type

Sub

DataType

Lethality Effect Level



LOAEL

Rep



NOEL

Rep



NOAEL

Rep



NOEL

Rep



NOAEL

Rep



NOAEL

Ref

(SR

Hazard

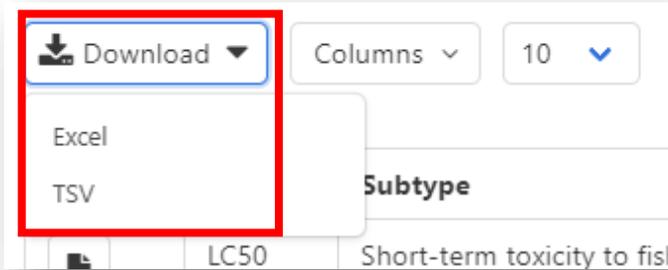
Human Eco

Hazard

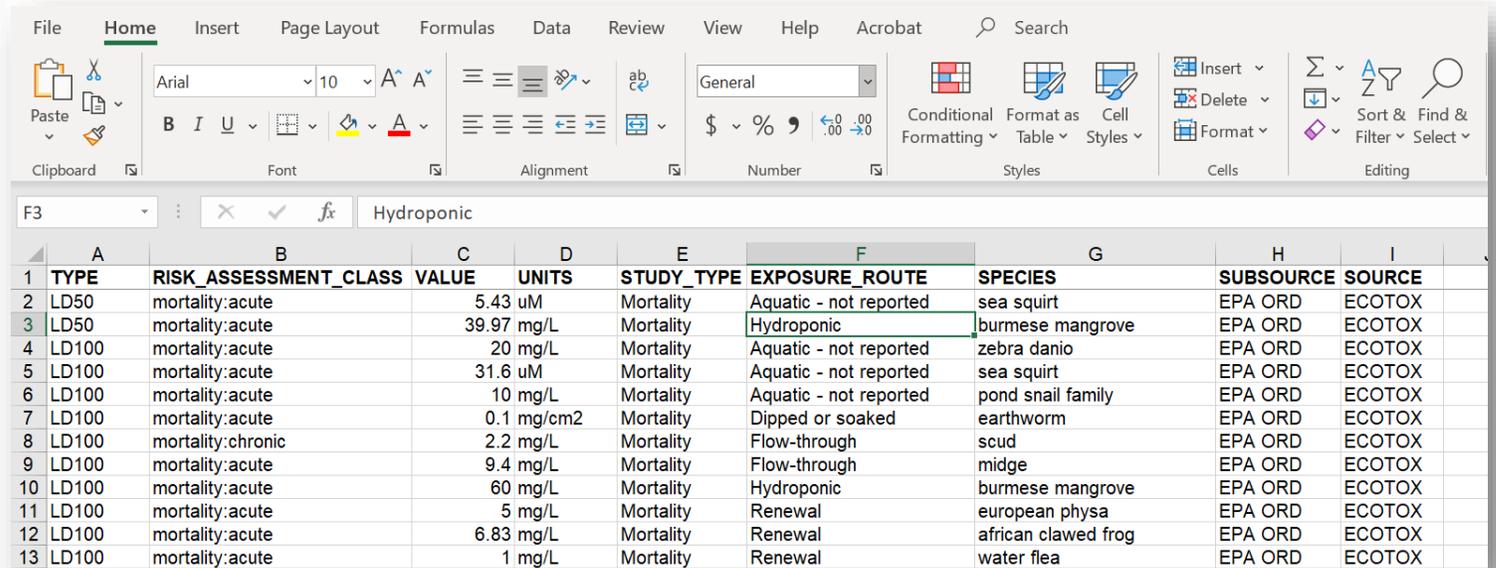
Human Eco

More	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	LC50	Short-term toxicity to fish	acute	35	mg/L	static	-	rainbow trout	eChemPortal	ECHA
	LC50	Short-term toxicity to fish	acute	4.6	mg/L	flow-through	-	fathead minnow	eChemPortal	ECHA
	LC50	Short-term toxicity to fish	acute	4.7	mg/L	flow-through	-	fathead minnow	eChemPortal	ECHA
	LC50	Short-term toxicity to fish	acute	9.4	mg/L	flow-through	-	atlantic silverside	eChemPortal	ECHA
	LC50	Short-term toxicity to fish	acute	15	mg/L	static	-	japanese medaka	eChemPortal	ECHA
	LC50	Short-term toxicity to fish	acute	11	mg/L	flow-through	-	sheepshead minnow	eChemPortal	ECHA

- Data are harvested from > 30 data sources and provides both human and ecological data for >50,000 chemicals



- General Feature** – anywhere you see a table you can download the data...



	A	B	C	D	E	F	G	H	I
1	TYPE	RISK_ASSESSMENT_CLASS	VALUE	UNITS	STUDY_TYPE	EXPOSURE_ROUTE	SPECIES	SUBSOURCE	SOURCE
2	LD50	mortality:acute	5.43	uM	Mortality	Aquatic - not reported	sea squirt	EPA ORD	ECOTOX
3	LD50	mortality:acute	39.97	mg/L	Mortality	Hydroponic	burmese mangrove	EPA ORD	ECOTOX
4	LD100	mortality:acute	20	mg/L	Mortality	Aquatic - not reported	zebra danio	EPA ORD	ECOTOX
5	LD100	mortality:acute	31.6	uM	Mortality	Aquatic - not reported	sea squirt	EPA ORD	ECOTOX
6	LD100	mortality:acute	10	mg/L	Mortality	Aquatic - not reported	pond snail family	EPA ORD	ECOTOX
7	LD100	mortality:acute	0.1	mg/cm2	Mortality	Dipped or soaked	earthworm	EPA ORD	ECOTOX
8	LD100	mortality:chronic	2.2	mg/L	Mortality	Flow-through	scud	EPA ORD	ECOTOX
9	LD100	mortality:acute	9.4	mg/L	Mortality	Flow-through	midge	EPA ORD	ECOTOX
10	LD100	mortality:acute	60	mg/L	Mortality	Hydroponic	burmese mangrove	EPA ORD	ECOTOX
11	LD100	mortality:acute	5	mg/L	Mortality	Renewal	european physa	EPA ORD	ECOTOX
12	LD100	mortality:acute	6.83	mg/L	Mortality	Renewal	african clawed frog	EPA ORD	ECOTOX
13	LD100	mortality:acute	1	mg/L	Mortality	Renewal	water flea	EPA ORD	ECOTOX

- Safety Data (Global Harmonization System (GHS)) from PubChem

GHS Data

Print Page

PUBCHEM > BISPHENOL A > LABORATORY CHEMICAL SAFETY SUMMARY (LCSS) > GHS CLASSIFICATION

CID 6623

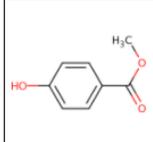
Bisphenol A

GHS Classification ?

Showing 6 of 6

Pictogram(s)	   Corrosive Irritant Health Hazard
Signal	Danger
GHS Hazard Statements	H317: May cause an allergic skin reaction [Warning Sensitization, Skin] H318: Causes serious eye damage [Danger Serious eye damage/eye irritation] H335: May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation] H360F: May damage fertility [Danger Reproductive toxicity]
Precautionary Statement Codes	P201, P202, P261, P271, P272, P280, P281, P302+P352, P304+P340, P305+P351+P338, P308+P313, P310, P312, P321, P333+P313, P363, P403+P233, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)

Sources of Exposure to Chemicals (More later – Kristin Isaacs)

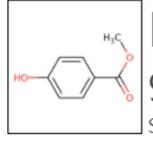


Methylparaben

99-76-3 | DTXSID4022529
Searched by DSSTox Substance Id.

Product and Use Categories (PUCs) i

Download Columns 10 Search query



Methylparaben

99-76-3 | DTXSID4022529
Searched by DSSTox Substance Id.

Chemical Weight Fractions i

Download Columns 25 Search query

Product Name	Product Use Category	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source
YOUTOPIA- PET SHAMPOO	all pets: pet shampoo			MSDS	CPCPdb
YLP Lip Gloss Solid F4203-06006-A12	make-up and related: lip gloss			MSDS	CPCPdb
ylp lip gloss liquid multiple colors 2	make-up and related: lip gloss			MSDS	CPCPdb
YLP Lip Gloss Liquid F4204-06001-A47	make-up and related: lip gloss			MSDS	CPCPdb
YLP Lip Gloss Liquid F4204-06001-A21	make-up and related: lip gloss			MSDS	CPCPdb
wondermask p peelable mask_ 2211 bulk	Not Yet Categorized:	0.00	1.00e-2	MSDS	SIRI
waterlss skn cleansr w/plastic scrubr_sbs-33	Not Yet Categorized:			MSDS	SIRI
water for injection_ bacteriostatic	Not Yet Categorized:			MSDS	SIRI
Water Based Nail Polish - 196C	nails: nail polish			other	CPCPdb
Washable Ink	Not Yet Categorized:			MSDS	CPCPdb
Vitamin Cream	facial cleansing and moisturizing: face cream/moisturizer			MSDS	CPCPdb

General Feature

On-hover Informational Icons

- Watch out for the on-hover informational icons to gather info

Source Id.

Product and Use Categories (PUCs)

The following papers are recommended reading. In regards to the categorization 'PUC' read [K. Isaacs et al, 2019, Journal of Exposure Science & Environmental Epidemiology](#). In regards to the CPCat cassette category read [K Dionisio et al 2015, Toxicology Reports](#). Please note the CPCat cassettes presented here are an updated version of those in the paper however application and interpretation of cassettes remains the same.

<u>Categorization type</u>	<u>Number of Unique Products</u>
----------------------------	----------------------------------

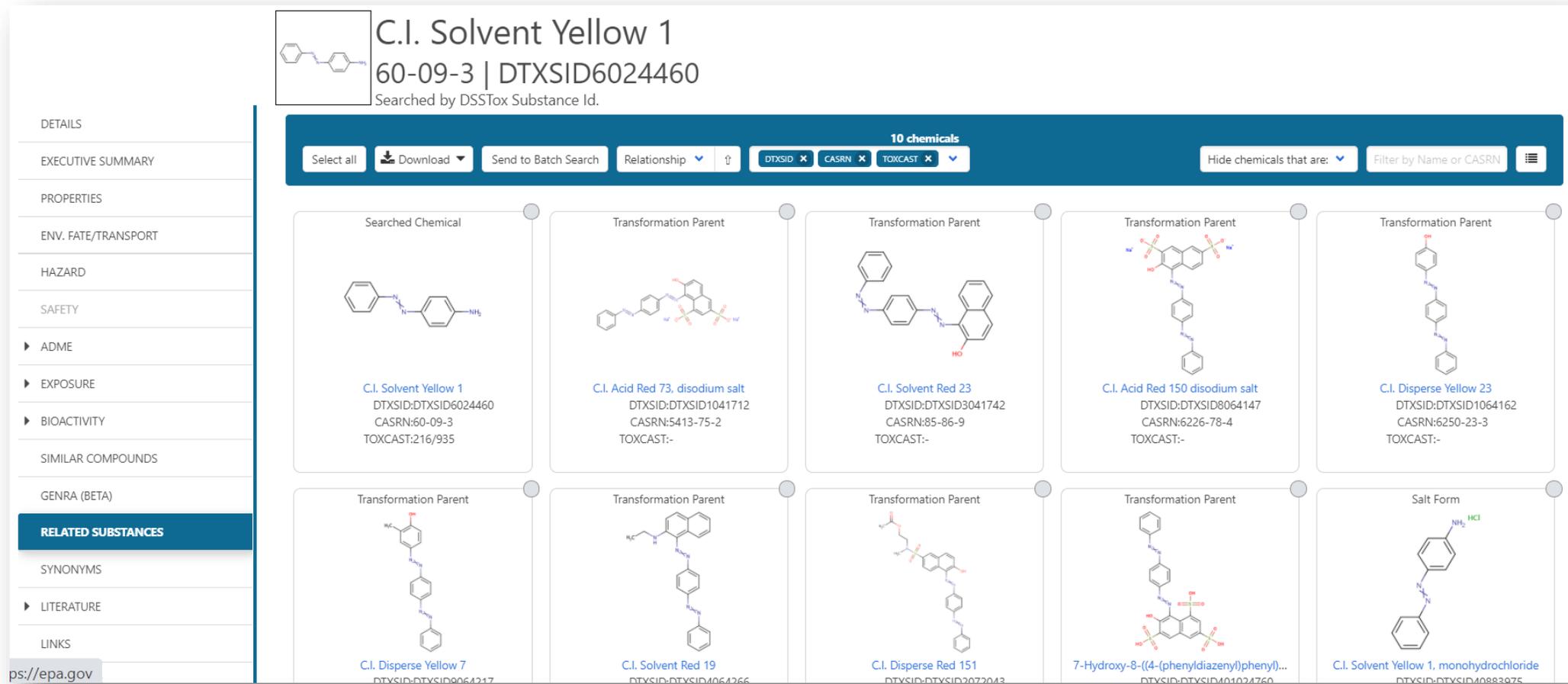
- Descriptive text or video about the data, associated publications etc.

Advanced Search capabilities presently support mass spectrometry at this point with mass and formula searching. For an overview of capabilities we recommend you watch [this short video](#). 

Related Substances

e.g. Aromatic amine to Azo Dyes

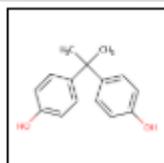
- Related substances – Parent to Transformation product: metabolites, degradants; Monomer to polymer;



The screenshot shows the EPA DSSTox Substance Id. interface for C.I. Solvent Yellow 1 (DTXSID:DTXSID6024460, CASRN:60-09-3). The interface includes a sidebar with navigation options like DETAILS, EXECUTIVE SUMMARY, PROPERTIES, ENV. FATE/TRANSPORT, HAZARD, SAFETY, ADME, EXPOSURE, BIOACTIVITY, SIMILAR COMPOUNDS, GENRA (BETA), RELATED SUBSTANCES (highlighted), SYNONYMS, LITERATURE, and LINKS. The main content area displays a grid of 10 related chemicals, categorized as Searched Chemical, Transformation Parent, or Salt Form. Each entry includes a chemical structure, name, and identifiers.

Category	Chemical Name	DTXSID	CASRN	TOXCAST
Searched Chemical	C.I. Solvent Yellow 1	DTXSID:DTXSID6024460	60-09-3	216/935
Transformation Parent	C.I. Acid Red 73, disodium salt	DTXSID:DTXSID1041712	5413-75-2	-
Transformation Parent	C.I. Solvent Red 23	DTXSID:DTXSID3041742	85-86-9	-
Transformation Parent	C.I. Acid Red 150 disodium salt	DTXSID:DTXSID8064147	6226-78-4	-
Transformation Parent	C.I. Disperse Yellow 23	DTXSID:DTXSID1064162	6250-23-3	-
Transformation Parent	C.I. Disperse Yellow 7	DTXSID:DTXSID8064217	-	-
Transformation Parent	C.I. Solvent Red 19	DTXSID:DTXSID4064266	-	-
Transformation Parent	C.I. Disperse Red 151	DTXSID:DTXSID2072043	-	-
Transformation Parent	7-Hydroxy-8-((4-(phenyldiazenyl)phenyl)...	DTXSID:DTXSID401024760	-	-
Salt Form	C.I. Solvent Yellow 1, monohydrochloride	DTXSID:DTXSID40883975	-	-

Identifiers to Support Searches



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.

Download

25

Search query

Synonyms

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

DETAILS

EXECUTIVE SUMMARY

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ENV. FATE/TRANSPORT

HAZARD

▶ ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

▶ LITERATURE

LINKS

COMMENTS

Identifiers to Support Searches

- Identifiers include systematic names, trade names, CASRNs (Active, Alternate and Deleted)

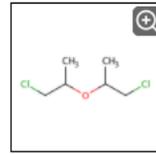
Synonym	Quality
beta,beta'-Bis(p-hydroxyphenyl)propane	Other
beta,beta-Di-(p-hydroxyphenyl)propane	Other
beta-Di-(p-hydroxyphenyl)propane	Other
beta-Di-p-hydroxyphenylpropane	Other
137885-53-1 Deleted CAS-RN	Deleted
146479-75-6 Deleted CAS-RN	Deleted
27360-89-0 Deleted CAS-RN	Deleted
28106-82-3 Deleted CAS-RN	Deleted
37808-08-5 Deleted CAS-RN	Deleted

<< < 1 2 3 4 5 6 > >>

Showing 126 to 134 of 134 records

Identifiers are used in the app

- Identifiers are used to feed and link into “Literature”



bis(2-Chloro-1-methylethyl) ether
108-60-1 | DTXSID4020167

▼ LITERATURE

- GOOGLE SCHOLAR
- PUBMED ABSTRACT SIFTER
- PUBCHEM ARTICLES
- PUBCHEM PATENTS
- PPRTV
- IRIS

IRIS [Contact Us](#)

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- IRIS Assessments**
- Advanced Search
- IRIS Program Materials
- Contact Us

Bis(2-chloro-1-methylethyl) ether

CASRN 108-60-1 | DTXSID4020167

- [IRIS Summary \(PDF\)](#) (7 pp, 91 K)

Key IRIS Values | Other EPA Information

Noncancer Assessment

[Reference Dose for Oral Exposure \(RfD\) \(PDF\)](#) (7 pp, 91 K) Last Updated: 10/01/1989

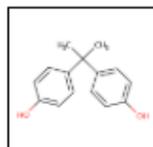
System	RfD (mg/kg-day)	Basis	PoD	Composite UF
Hematologic	4 x 10 ⁻²	Decrease in hemoglobin and ...	NOAEL : 3.58 x 10 ¹	1000

Related Links

- [EPA Chemicals Dashboard - Bis\(2-chloro-1-methylethyl\) ether](#)

Critical Effect Systems

External Links – Also use Identifiers Names, CASRN, PubChem IDs...



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.

DETAILS

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▶ BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

▶ LITERATURE

LINKS

COMMENTS

General

-  EPA Substance Registry Service
-  Household Products Database
-  Chemical Entities of Biological Interest (ChEBI)
-  PubChem
-  Chempider
-  CPCat
-  DrugBank
-  HMDB
-  Wikipedia
-  MSDS Lookup
-  ChEMBL
-  Chemical Vendors
-  CalEPA Office of Environmental Health Hazard Assessment
-  NIOSH Chemical Safety Cards
-  ToxPlanet
-  ACS Reagent Chemicals
-  Wikidata
-  ChemHat: Hazards and Alternatives Toolbox
-  Wolfram Alpha
-  ScrubChem
-  ECHA Brief Profile

Toxicology

-  ACToR
-  DrugPortal
-  CCRIS
-  ChemView
-  CTD
-  eChemPortal
-  Gene-Tox
-  HSDB
-  ToxCast Dashboard 2
-  LactMed
-  International Toxicity Estimates for Risk
-  ATSDR Toxic Substances Portal
-  Superfund Chemical Data matrix
-  NIOSH IDLH Values
-  ACToR PDF Report
-  Toxics Release Inventory
-  CREST
-  National Air Toxics Assessment

Publications

-  Toxline
-  Environmental Health Perspectives
-  NIEHS
-  National Toxicology Program
-  Google Books
-  Google Scholar
-  Google Patents
-  PPRTVWEB
-  PubMed
-  IRIS Assessments
-  EPA HERO
-  NIOSH Skin Notation Profiles
-  NIOSH Pocket Guide
-  RSC Publications
-  BioCaddie DataMed
-  Springer Materials
-  Federal Register
-  Regulations.gov
-  Bielefeld Academic Search Engine
-  CORE Literature Search

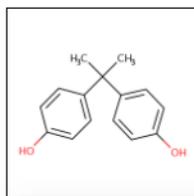
Analytical

-  FOR-IDENT
-  NEMI: National Environmental Methods Index
-  RSC Analytical Abstracts
-  Tox21 Analytical Data
-  MONA: MassBank North America
-  mzCloud
-  NIST NIST IR Spectrum
-  NIST NIST MS Spectrum

Prediction

-  2D NMR HSQC/HMBC Prediction
-  Carbon-13 NMR Prediction
-  Proton NMR Prediction
-  ChemRTP Predictor
-  LSERD

External Links



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

General



Service

 PubChem

 Chemspider

 CPCat

 DrugBank

 Wikipedia

 MSDS Lookup

 ChEMBL

 ToxPlanet

 ACS Reagent Chemicals

 ChemHat: Hazards and Alternatives Toolbox

Toxicology

 ACToR

 DrugPortal

 CCRIS

 ChemView

 CTD

 eChemPortal

 Gene-Tox

 HSDB

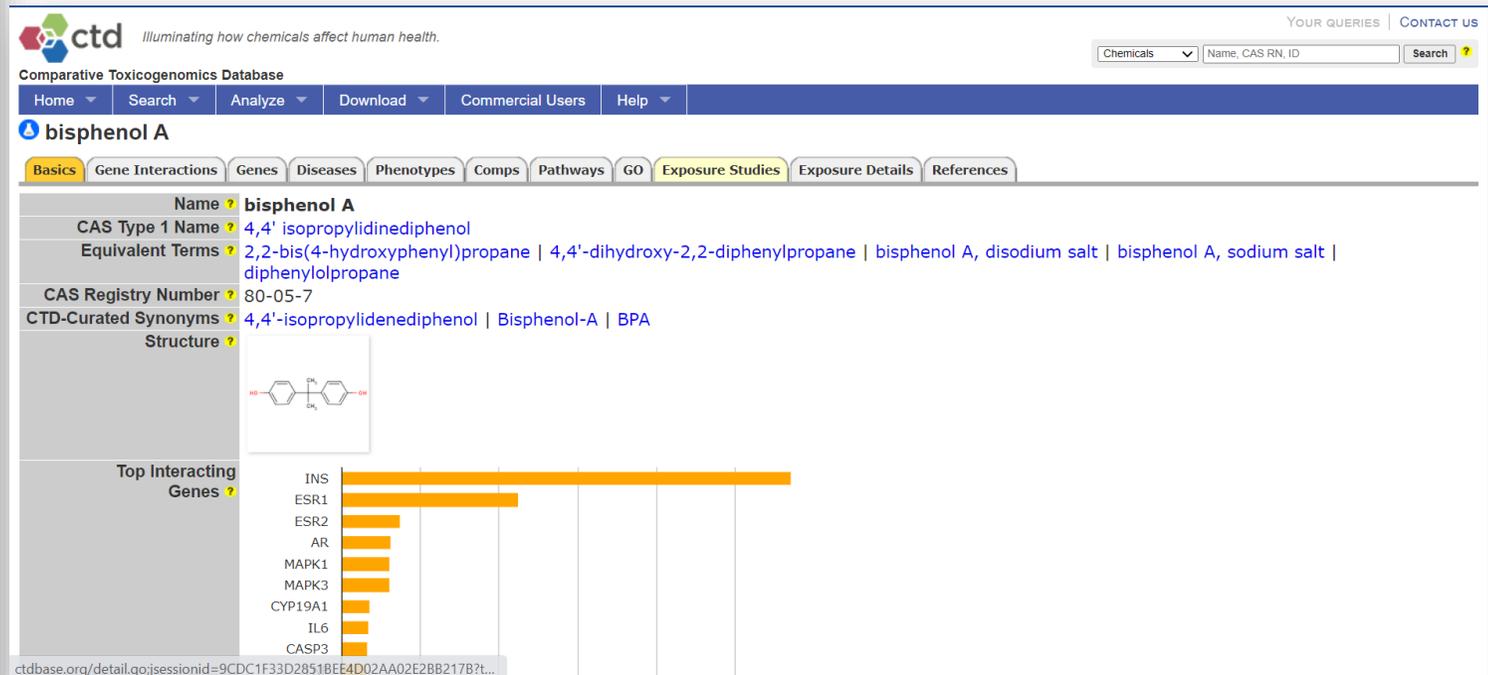
 ToxCast Dashboard 2

 ACToR PDF Report

 CREST

 National Air Toxics Assessment

- Links to ~90 websites providing access to additional data on the chemical of interest



ctd Illuminating how chemicals affect human health.

YOUR QUERIES | CONTACT US

Chemicals | Name, CAS RN, ID | Search

Comparative Toxicogenomics Database

Home | Search | Analyze | Download | Commercial Users | Help

bisphenol A

Basics | Gene Interactions | Genes | Diseases | Phenotypes | Comps | Pathways | GO | Exposure Studies | Exposure Details | References

Name **bisphenol A**

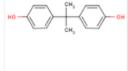
CAS Type 1 Name **4,4' isopropylidenediphenol**

Equivalent Terms **2,2-bis(4-hydroxyphenyl)propane | 4,4'-dihydroxy-2,2-diphenylpropane | bisphenol A, disodium salt | bisphenol A, sodium salt | diphenylolpropane**

CAS Registry Number **80-05-7**

CTD-Curated Synonyms **4,4'-isopropylidenediphenol | Bisphenol-A | BPA**

Structure

CC1(C)C=C(O)C=C1C2=CC=C(O)C=C2

Top Interacting Genes

Gene	Interaction Score
INS	100
ESR1	85
ESR2	75
AR	65
MAPK1	55
MAPK3	55
CYP19A1	45
IL6	40
CASP3	35

ctdbase.org/detail.go?jsessionid=9CDC1F33D2851BE4D02AA02E2BB217B?t...

More details will be covered on...

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

- ADME:IVIVE will be covered by John Wambaugh
- Exposure will be covered by Kristin Isaacs
- Bioactivity will be covered by Katie Paul-Friedman
- GenRA will be covered by Grace Patlewicz
- Literature:Abstract Sifter will be covered by Nancy Baker
- ...and much of this data will show up in the Executive Summary for a chemical substance

Executive Summary

Summary view of relevant data

Quantitative Risk Assessment Values

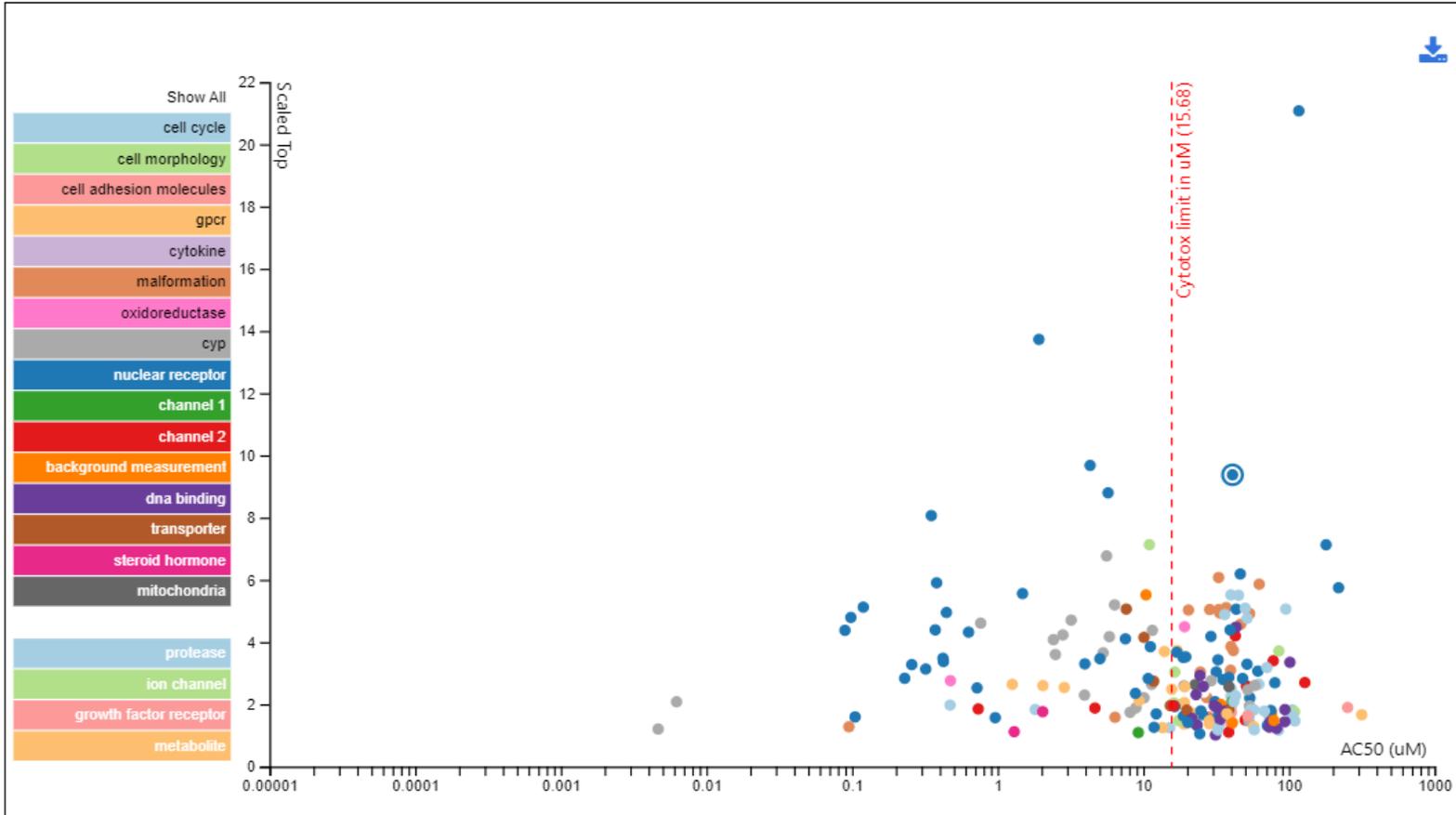
✓ IRIS values available [↗](#)

Endocrine System

✓ Endocrine Disruption Potential. Significant Estrogen and Androgen Receptor activity seen. Chemical was positive

TOXCAST DATA

ASSAY DETAILS



AC50 (uM): 40.99
Scaled top: 9.38
Assay Endpoint Name: ACEA_AR_antagonist_80hr
Gene Symbol: AR
Organism: human
Tissue: prostate
Assay Format Type: cell-based
Biological Process Target: cell proliferation
Detection Technology: RT-CES
Analysis Direction: NA
Intended Target Family: nuclear receptor
Description: Data from the assay component ACEA_AR_agonist_80hr was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of growth reporter, measures of the cells for gain-of-signal activity can be used to understand the signaling at the pathway-level as they relate to the gene AR. Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced multiple assay endpoints where this one serves a signaling function. 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".

Developmental Toxicology

✓ Developmental toxicity PODs available [↗](#)

logP

log(BCF)

log(VP)

Advanced Searching: Mass and Formula

Advanced Searches

Mass and Formula Searches

Supports our suspect screening and non-targeted analysis mass spectrometry research efforts

Mass Search

Min/Max

Adduct: Neutral  All Adducts Choose adduct from dropdown

Da Da ppm



Molecular Formula Search

MS Ready Formula  Exact Formula 

Formula

Please use the format of the following example: C6H8O2 or C6H(8-10)O(0-2)

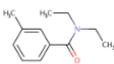
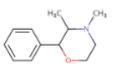
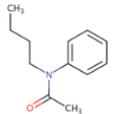
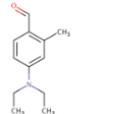
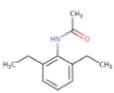
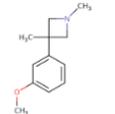
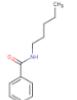
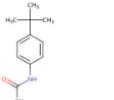
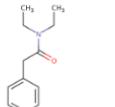
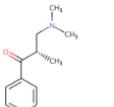
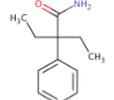
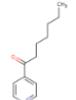


Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

329 of 329 chemicals visible

Select all

 <p>DEET DTXSID: DTXSID2021995 CASRN: 134-62-3 TOXCAST: 12768 Mass Diff: 0.000014</p>	 <p>Phendimetrazine DTXSID: DTXSID1023447 CASRN: 634-03-7 TOXCAST: - Mass Diff: 0.000014</p>	 <p>N-Butylacetanilide DTXSID: DTXSID2042197 CASRN: 91-49-6 TOXCAST: - Mass Diff: 0.000014</p>	 <p>Benzaldehyde, 4-(diethylamino)-2-methyl- DTXSID: DTXSID4059041 CASRN: 92-14-8 TOXCAST: - Mass Diff: 0.000014</p>	 <p>Acetanilide, 2-(6-diethylamino-1,3-dimethyl-3-(m-methoxyphenyl)propyl)- DTXSID: DTXSID90168148 CASRN: 16665-89-7 TOXCAST: - Mass Diff: 0.000014</p>	 <p>Azetidine, 1,3-dimethyl-3-(m-methoxyphenyl)- DTXSID: DTXSID40173560 CASRN: 19832-26-9 TOXCAST: - Mass Diff: 0.000014</p>
 <p>Benzamide, N-pentyl- DTXSID: DTXSID20174196 CASRN: 20308-43-4 TOXCAST: - Mass Diff: 0.000014</p>	 <p>p-t-Butylacetanilide DTXSID: DTXSID60174238 CASRN: 20330-45-4 TOXCAST: - Mass Diff: 0.000014</p>	 <p>N,N-Diethylphenylacetamide DTXSID: DTXSID00179048 CASRN: 2431-96-1 TOXCAST: - Mass Diff: 0.000014</p>	 <p>3-(Dimethylamino)-2-methylpropylphenyl- DTXSID: DTXSID60180796 CASRN: 26171-50-6 TOXCAST: - Mass Diff: 0.000014</p>	 <p>Butyramide, 2-ethyl-2-phenyl- DTXSID: DTXSID60184653 CASRN: 30568-39-9 TOXCAST: - Mass Diff: 0.000014</p>	 <p>1-Heptanone, 1-(4-pyridyl)- DTXSID: DTXSID40186594 CASRN: 32941-30-3 TOXCAST: - Mass Diff: 0.000014</p>

Batch Searching

Access data *en masse* for thousands of chemicals.....

Batch Search ?



Step Three: Select Download Data or Display Chemicals

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 (One per line. Searches should be limited to <5000 identifiers.)

Sodium azide
O,O-Dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] phosphorodithioate
(Trichloromethyl)benzene
100-44-7
(Chloromethyl)benzene
98-07-7
111-44-4
1-Chloro-2-(2-chloroethoxy)ethane
Chloro(chloromethoxy)methane
2-(Butan-2-yl)-4,6-dinitrophenol

Display All Chemicals

Download Chemical Data

Select Output Format and Content

Step Four: Select Data Output Format and Choose Data Fields to Download

Select Output Format:

 Excel 

 Download

Customize Results

- Select All
- Select All in Lists

Chemical Identifiers

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

Structures

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

Intrinsic And Predicted Properties

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

Metadata

- Curation Level Details 
- NHANES/Predicted Exposure 
- Data Sources 
- Include ToxVal Data Availability 
- Assay Hit Count 
- Number of PubMed Articles 
- PubChem Data Sources 
- CPDat Product Occurrence Count 
- IRIS 
- PPRTV 
- Wikipedia Article
- QC Notes 
- Include links to ACToR reports - SLOW! (BETA) 

Presence in Lists:

- 40CFR116.4 Designation of Hazardous Substances (Above Ground Storage Tanks) 
- 40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities 
- AEGLs: Acute Exposure Guideline Levels 
- ANDROGEN: Androgen Receptor Chemicals 
- ARTICLE; Bench-Mark Dose Human Health Assessment List (Wignall et al., 2014) 
- ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (CERAPP) 
- ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (COMPARA) 
- ATSDR Toxicological Profiles 
- ATSDR: Minimal Risk Levels (MRLs) for Hazardous Substances 
- ATSDR: Toxic Substances Portal Chemical List 
- California Office of Environmental Health Hazard Assessment 
- Canadian Domestic Substances List 2019 
- CATEGORY: Amino acids 
- CATEGORY: Color Index dyes 
- CATEGORY: Flame Retardants 

Batch Search CASRN

Batch Search



Step Four: Select Data Output Format and Choose Data Fields to Download

Please enter one identifier per line

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
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- TEST Model Predictions
- OPERA Model Predictions

Metadata

- Curation Level Details
- NHANES/Predicted Exposure
- Data Sources
- Include ToxVal Data Availability
- Assay Hit Count
- Number of PubMed Articles

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	INPUT	FOUND_BY	DTXSID	PREFERRE	CASRN	INCHIKEY	IUPAC_NAI	MOLECULA	TOXVAL_D	TOXCAST	TOXCAST	MS_READY	NUMBER_CIRIS	LINK	PPRTV	LINATMOSPHE	BIOCONCE
2	534-52-1	CAS-RN	DTXSID10	2-Methyl-4,	534-52-1	ZXVONLUN	2-Methyl-4,	C7H6N2O5	Y	27.56	261/947	CC1=C(O)C	179	-	Y	1.571E-12	2.88959
3	115-21-9	CAS-RN	DTXSID70	Ethyl silicon	115-21-9	ZOYFEXPF	Trichloro(etr	C2H5Cl3Si	Y	-	-	-	-	-	-	8.289E-12	13.9658
4	111-44-4	CAS-RN	DTXSID90	Bis(2-chloro	111-44-4	ZNSMNVML	1-Chloro-2-(C4H8Cl2O	Y	1.12	10/891	CICCOCCC	12	Y	-	2.647E-12	9.99608
5	2763-96-4	CAS-RN	DTXSID50	Muscimol	2763-96-4	ZJQHPWUV	5-(Aminome	C4H6N2O2	Y	-	-	NCC1=CC(C	4308	-	-	1.179E-10	5.05695
6	1464-53-5	CAS-RN	DTXSID00	2,2'-Bioxiran	1464-53-5	ZFIVKAOQ	2,2'-Bioxiran	C4H6O2	Y	-	-	C1OC1C1C	363	-	-	4.383E-12	1.27107
7	22224-92-6	CAS-RN	DTXSID30	Fenamiphos	22224-92-	ZCJPOBZI	Ethyl 3-metr	C13H22NO3	Y	10.8	105/972	CCOP(=O)(58	Y	-	1.66E-11	2.3394
8	359-06-8	CAS-RN	DTXSID40	Fluoroacetyl	359-06-8	ZBHDTYQJ	Fluoroacetyl	C2H2ClFO	Y	-	-	FCC(Cl)=O	-	-	-	3.513E-13	4.49379
9	5344-82-1	CAS-RN	DTXSID40	1-(o-Chloro	5344-82-1	YZUKKTCD	N-(2-Chloro	C7H7ClN2S	Y	-	-	NC(=S)NC1-	-	-	-	2.482E-11	9.95206
10	7446-18-6	CAS-RN	DTXSID10	Thallium (I)	7446-18-6	YTQVHRVI	Dithallium(1-	O4STI2	Y	-	-	-	34	Y	Y	-	-
11	62207-76-5	CAS-RN	DTXSID40	Bis(3-fluoro	62207-76-	YRZXYIHD	-	C16H14CoF	Y	-	-	-	-	-	-	-	-
12	66-81-9	CAS-RN	DTXSID60	Cycloheximi	66-81-9	YPHMISFO	4-{(2R)-2-[(C15H23NO4	Y	32.27	294/911	CC1CC(C)C	18709	-	-	1.756E-11	2.81761
13	106-96-7	CAS-RN	DTXSID30	Propargyl bi	106-96-7	YORCIIVHU	3-Bromopro	C3H3Br	Y	-	-	BrCC#C	-	-	-	1.069E-11	10.4968
14	315-18-4	CAS-RN	DTXSID70	Mexacarbat	315-18-4	YNEVBPNI	4-(Dimethyl	C12H18N2C	Y	5.11	12/235	CNC(=O)OC	27	-	-	1.447E-11	26.2914
15	110-00-9	CAS-RN	DTXSID60	Furan	110-00-9	YLQBMQCI	Furan	C4H4O	Y	0.0	0/235	O1C=CC=C	919	Y	-	4.019E-11	5.01648
16	3037-72-7	CAS-RN	DTXSID20	4-(diethoxyn	3037-72-7	YHFFINXFN	4-[Diethoxy	C9H23NO2S	Y	-	-	-	-	-	-	5.95E-12	6.71292
17	75-44-5	CAS-RN	DTXSID00	Phosgene	75-44-5	YGYAWVD	Carbonyl dic	CCl2O	Y	-	-	ClC(Cl)=O	489	Y	-	9.994E-16	13.0711
18	2032-65-7	CAS-RN	DTXSID30	Methiocarb	2032-65-7	YFBPRJGD	3,5-Dimethy	C11H15NO2	Y	18.14	88/485	CNC(=O)OC	65	-	-	1.446E-11	34.1692
19	2778-04-3	CAS-RN	DTXSID20	Endothion	2778-04-3	YCAGGFXS	S-[(5-Metho	C9H13O6P3	Y	-	-	COC1=COCC	-	-	-	4.355E-11	1.18341
20	12108-13-3	CAS-RN	DTXSID90	(Methylcyclo	12108-13-	YASXMYPV	Tricarbonyl	C9H7MnO3	Y	2.56	11/430	-	68	-	-	-	-
21	7803-51-2	CAS-RN	DTXSID20	Phosphine	7803-51-2	XYFCBTPG	Phosphane	H3P	Y	-	-	-	928	Y	-	-	-
22	107-18-6	CAS-RN	DTXSID80	Allyl alcohol	107-18-6	XXROGKLT	Prop-2-en-1	C3H6O	Y	3.99	17/426	OCC=C	627	Y	Y	2.592E-11	4.03901
23	108-05-4	CAS-RN	DTXSID30	Vinyl acetat	108-05-4	XTXRWKR	Ethethyl acel	C4H6O2	Y	1.7	4/235	CC(=O)OC-	206	Y	-	2.5E-11	5.52157
24	19624-22-7	CAS-RN	DTXSID10	Pentaborane	19624-22-	XPIBKKWN	-	B5H9	Y	-	-	-	-	-	-	-	-
25	75-74-1	CAS-RN	DTXSID00	Tetramethyl	75-74-1	XOOGZRUE	Tetramethyl	C4H12Pb	Y	-	-	C[Pb](C)(C)	24	-	-	-	-

How Can You Help?

How can you help?

- Please submit comments for curation and feedback. We will respond.

New Comment

Comment

I am looking at [peroxybenzoylnitrate](#). The dashboard tells me that the molecules with a methyl group on the benzene ring either meta or para have a similarity of 1 to the molecule (that has no methyl group) but a methyl [ortho](#) has a lower similarity.

Email address

I'm not a robot



Submit

Crowdsourced Comments

25 ▼

Search query

Chemical	Structure	Date	Comment	Resolution
Didecyldimethylammonium chloride		2020-10-11	I don't think the "Product Use Category" sorting function (on table) is working. The other columns seem to work.	Resolved
Carotenoids	No Chemical Structure Associated with this Substance	2020-10-11	36-88-4 is not a CASRN	Resolved
2-(Dimethylamino)-1-phenylethanol		2020-10-07	This entry is a rare instance of disagreement for CASRN between EPA Chemistry Dashboard and ChemIDplus. ChemIDplus associates CASRN 99614-01-4 with Ondansetron hydrochloride: https://chem.nlm.nih.gov/chemidplus/rn/99614-01-4 Could someone check and let me know which is correct? Thanks, AAB	Resolved
2-Hexenal, 5-methyl-2-(1-methylethyl)-		2020-09-25	Isodihydroavandulyl aldehyde BAD spelling lacks letter l - also present correctly ! IUPAC name 2-isopropyl-5-methylhex-2-enal RTECS is MP6450000 REAXYS/BRN is 1752384 Several other corrections ! 2-Hexen-1-al, 5-methyl-2-(1-methylethyl)- is a muddle of IUPAC & CAS names - remove ?? Barrie	Resolved
2-Hexenal, 5-methyl-2-(1-methylethyl)-		2020-09-25	Isodihydroavandulyl aldehyde BAD spelling lacks letter l - also present correctly ! IUPAC name 2-isopropyl-5-methylhex-2-enal RTECS is MP6450000 REAXYS/BRN is 1752384 Several other corrections ! 2-Hexen-1-al, 5-methyl-2-(1-methylethyl)- is a muddle of IUPAC & CAS names - remove ?? Barrie	Resolved

Prototypes in Progress

PROTOTYPE Structure/Substructure/Similarity Search available

Search Atrazine

6-Chloro-1,3,5-triazine-2,4-diamine 3397-62-4 DTXSID1037806

Search

- Exact
- Substructure
- Similarity
- Molecular Formula
- Molecular Weight
- Features

Min similarity: 0.5

Similarity-type: Tanimoto

Stereo Chiral Isotopes Charged Multicomponent Radicals Salts

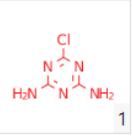
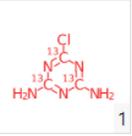
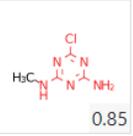
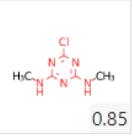
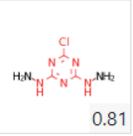
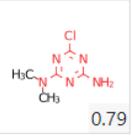
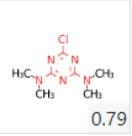
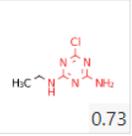
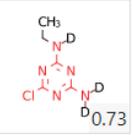
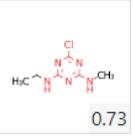
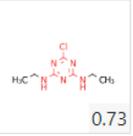
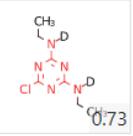
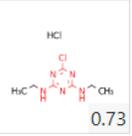
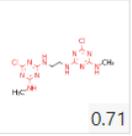
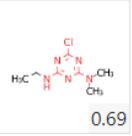
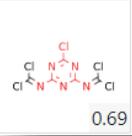
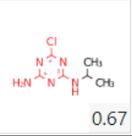
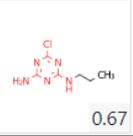
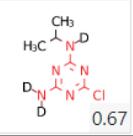
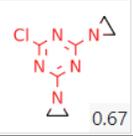
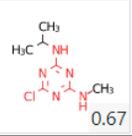
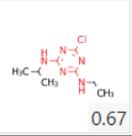
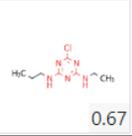
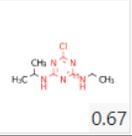
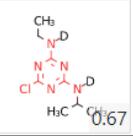
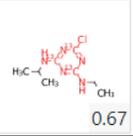
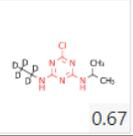
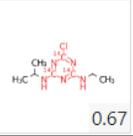
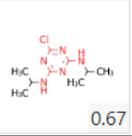
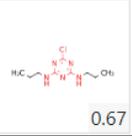
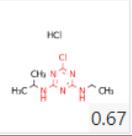
Polymers Sgroups

Elements must be included: e.g. C,F,H

Elements must be excluded: e.g. C,F,H

Found 133 records containing the following elements: C, Cl, H, N, O

Stereo Chiral Isotopes (14) Charged Multicomponent (7) Radicals Salts Polymers Sgroups Sort Similarity

 1	 1	 0.85	 0.85	 0.81	 0.79	 0.79	 0.73	 0.73	 0.73	 0.73	 0.73	 0.73	 0.73	 0.71	 0.69
 0.69	 0.67	 0.67	 0.67	 0.67	 0.67	 0.67	 0.67	 0.67	 0.67	 0.67	 0.67	 0.67	 0.67	 0.67	 0.67

PROTOTYPE Hazard Comparison Dashboard

The Hazard Comparison Dashboard is a prototype tool and a compilation of information sourced from many sites, databases and sources including U.S. Federal and state sources and international bodies that saves the user time by providing information in one location. The data are not reviewed by USEPA – the user must apply judgment in use of the information. The results do not indicate EPA's position on the use or regulation of these chemicals.

Hazard Comparison Dashboard

Hazard

Predict

Search

Standardizer

Hazard Comparison

None

Export



169 / 169



Legend: **VH** - Very High, **H** - High, **M** - Medium, **L** - Low, **I** - Inconclusive **Authoritative**, Screening, QSAR Model

CAS Name	Human Health Effects										Ecotoxicity		Fate						
	Acute Mammalian Toxicity			Carcinogenicity	Genotoxicity/Mutagenicity	Endocrine Disruption	Reproductive	Developmental	Neurotoxicity		Systemic Toxicity		Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation
	Oral	Inhalation	Dermal						Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure							
75-05-8 Acetonitrile	M	M	M	I	L	L	I	L	M	M	M	M	M	L	M	L	M	M	M
107-02-8 Acrolein	VH	VH	H	H	H	L	L	L	M	M	M	M	M	L	M	L	M	M	M
107-13-1 Acrylonitrile	H	H	H	VH	H	L	H	H	M	M	M	M	M	L	M	L	M	M	M
107-18-6 Allyl alcohol	H	H	H	H	L	H	I	I	M	M	M	M	M	L	M	L	M	M	M
62-53-3 Aniline	H	H	H	VH	H	L	M	L	M	M	M	M	M	L	M	L	M	M	M

- Skipped (1)
- Filters (0)
- Sorting (0)
- Products (0)
- Structure

 Springer Link

Original Paper | Published: 21 January 2020

An automated framework for compiling and integrating chemical hazard data

[Leora Vegosen](#) & [Todd M. Martin](#) 

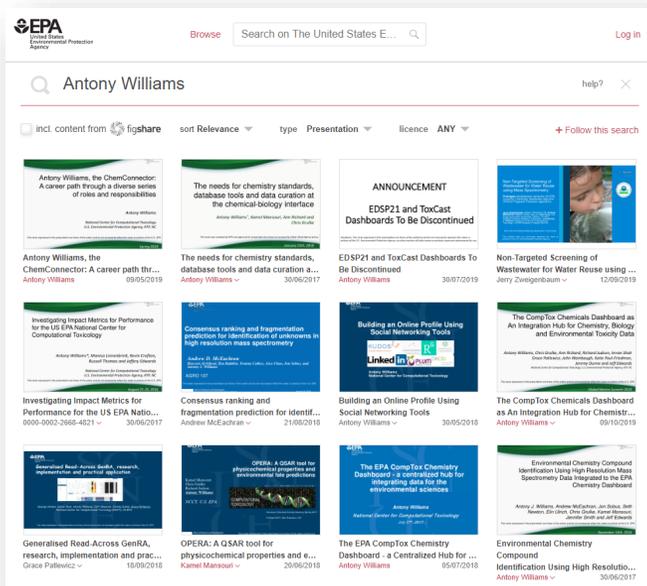
[Clean Technologies and Environmental Policy](#) **22**, 441–458(2020) | [Cite this article](#)

163 Accesses | [Metrics](#)

Online Materials

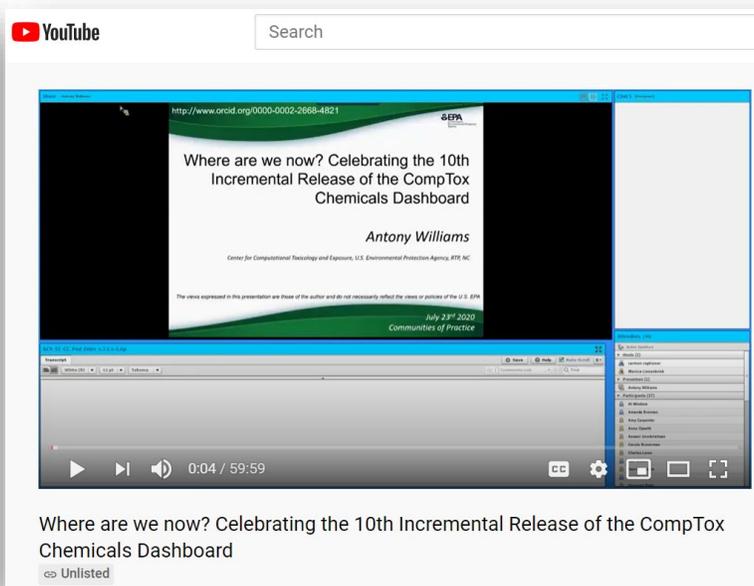
You want to know more...

- Lots of resources available
 - Presentations: <https://tinyurl.com/w5hq55>
 - Communities of Practice Videos: <https://rb.gy/qsbn01>
 - Manual: <https://rb.gy/4fgydc>
 - Latest News: https://comptox.epa.gov/dashboard/news_info



Search results for 'Antony Williams' on the EPA website. The results are sorted by Relevance and include various presentations and documents. Key items include:

- Antony Williams, the ChemConnector: A career path through a diverse series of roles and responsibilities
- The needs for chemistry standards, database tools and data curation at the chemical-biology interface
- ANNOUNCEMENT: EDS21 and ToxCast Dashboards To Be Discontinued
- Non-Targeted Screening of Wastewater for Water Reuse using ...
- Investigating Impact Metrics for Performance for the U.S. EPA National Center for Computational Toxicology
- Consensus ranking and fragmentation prediction for identification of unknowns in high resolution mass spectrometry
- Building an Online Profile Using Social Networking Tools
- The CompTox Chemicals Dashboard as an Integration Hub for Chemistry, Biology and Environmental Toxicity Data
- Investigating Impact Metrics for Performance for the US EPA National Center for Computational Toxicology
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- The CompTox Chemicals Dashboard as an Integration Hub for Chemistry, Biology and Environmental Toxicity Data
- Generalised Read Across GenRA, research, implementation and practice
- OPERA: A QSAR tool for physicochemical properties and environmental fate prediction
- The EPA CompTox Chemistry Dashboard - a Centralized Hub for ...
- Environmental Chemistry Compound Identification Using High Resolution Mass Spectrometry Data Integrated to the EPA Chemistry Dashboard



YouTube video player showing a presentation titled "Where are we now? Celebrating the 10th Incremental Release of the CompTox Chemicals Dashboard" by Antony Williams. The video is currently at 0:04 / 59:59. The presentation content includes the EPA logo, the title, the presenter's name, and the date "July 29th 2020 Communities of Practice".

Where are we now? Celebrating the 10th Incremental Release of the CompTox Chemicals Dashboard

Antony Williams

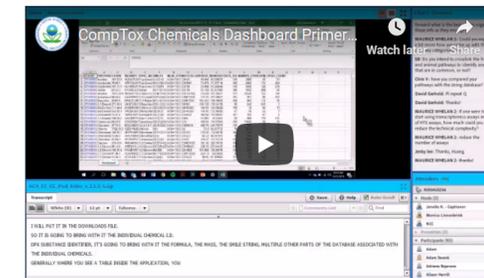
July 29th 2020
Communities of Practice

CompTox Chemicals Dashboard primer videos

The CompTox Chemicals Dashboard is a one-stop-shop for chemistry, toxicity and exposure information for over 875,000 chemicals. Data and models within the Dashboard also help with efforts to identify chemicals of most need of further testing and reducing the use of animals in chemical testing.

Explore the wealth of data and features available in the CompTox Chemicals Dashboard with these instructional videos narrated by EPA scientists.

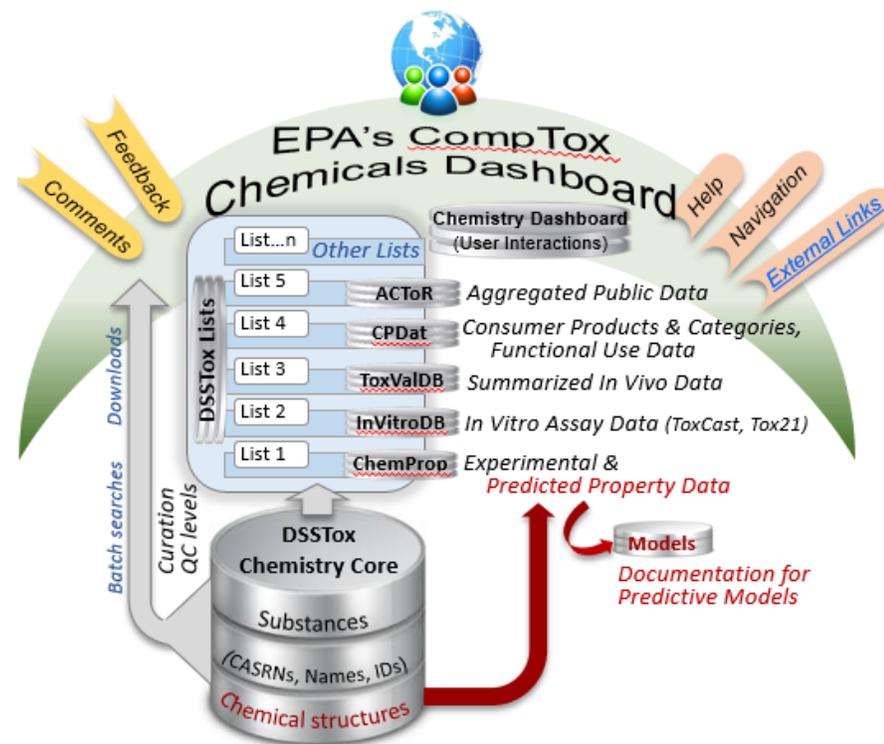
General Chemistry and Search Capabilities



Video player showing a primer video for the CompTox Chemicals Dashboard. The video displays a screenshot of the dashboard interface, which includes a search bar, a list of chemical entries, and various data columns. The video is titled "CompTox Chemicals Dashboard Primer" and includes a "Watch Later" button.

Conclusion

- Dashboard access to data for ~882,000 chemicals (and growing)
- Data aggregation for ALL data sources continues unabated
- Flexible search capabilities continue to expand release-to-release
- Expansion of new modules continues with prototype development
- The application is being totally rearchitected at present to also develop a Public API
- ...and now for the deeper dives into the relevant sub-tabs and modules...



Acknowledgments

- Contact: Williams.Antony@epa.gov
- Feedback and follow-up is welcomed! Your questions help
- The dashboard is based on the efforts of many more team members than us. Many collaborators provide data also.
- Thank you NURA for hosting us



EPA's Center for Computational Toxicology and Exposure