

US-EPA CompTox chemicals dashboard: A web-based data integration hub for environmental chemistry data

*Antony Williams, Chris Grulke, Richard Judson,
John Wambaugh, Jeremy Dunne and Jeff Edwards*

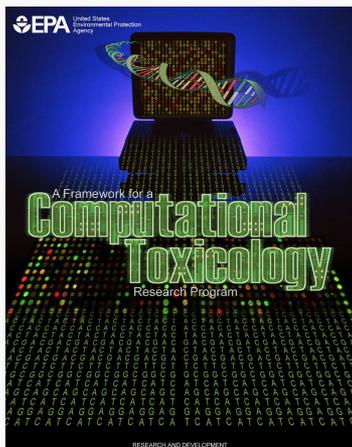
National Center for Computational Toxicology, U.S. Environmental Protection Agency, RTP, NC

The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA

*Spring 2019
ACS Spring Meeting, Orlando*

- The US EPA's CompTox Chemistry Dashboard provides access to various types of data associated with ~760,000 chemical substances. These data include experimental and predicted property data, high-throughput screening assay data and hazard and environmental exposure data. With millions of individual data points and annotations associated with hundreds of thousands of chemicals, data quality is a priority. With tens of thousands of individual users per month browsing the data on the dashboard, the ability of users to provide feedback has allowed us to identify, confirm and address issues in the data. This has required the implementation of novel approaches for data feedback via the user interface that include general feedback on the dashboard and down to individual data points contained in a table. We are presently investigating ways to garner feedback on our ToxCast bioassay data to facilitate the curation of tens of thousands of data points. This presentation will provide an overview of our existing capabilities in the CompTox Chemistry Dashboard for gathering crowdsourced data from the user base and its impact on assisting in the curation of data.

National Center for Computational Toxicology



- National Center for Computational Toxicology established in 2005 to integrate:
 - High-throughput and high-content technologies
 - Modern molecular biology
 - Data mining and statistical modeling
 - Computational biology and chemistry
- Researching computational approaches to quickly evaluate the safety of chemicals for potential risk.
- Outputs: a lot of data, models, algorithms and software applications

- A publicly accessible website delivering access:
 - New entry portal for all NCCT dashboards
 - ~**762,000** chemicals with related property data
 - **Searchable by chemical, product use, gene and assay (ToxCast)**
 - Experimental and predicted physicochemical property data
 - **“Bioactivity data” for the ToxCast/Tox21 project**
 - **Generalized Read-Across (GenRA) module**
 - Links to other agency websites and public data resources
 - “Literature” searches for chemicals using public resources
 - “Batch searching” for thousands of chemicals
 - **DOWNLOADABLE** Open Data for reuse and repurposing

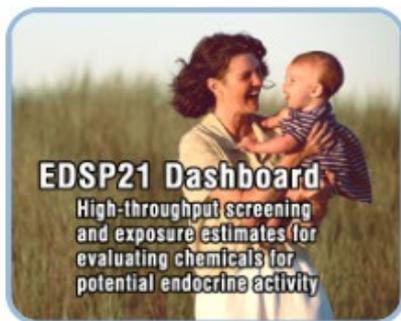
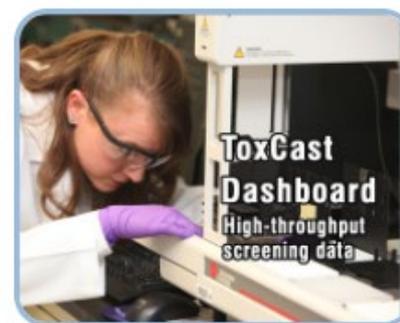
CompTox Portal

Environmental Topics

Laws & Regulations

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Data.gov

Inspector General

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Hotlines



Chemicals Product/Use Categories Assay/Gene

762 Thousand Chemicals

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](#)

Latest News

[Read more news](#)

YouTube video regarding using the Dashboard for Non-Targeted Analysis

March 7th, 2018 at 9:43:36 AM

Ar
Mar

YouTube video discussing the application of the CompTox Chemistry Dashboard to support non-targeted analysis by mass spectrometry is available. This short video summarizes the advantages of the dashboard in terms of data quality and focused data set for environmental non-targeted analysis. [View it here on Youtube.](#)



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CompTox Dashboard Chemicals

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share

762 Thousand Chemicals

Chemicals Product/Use Categories Assay/Gene

Q Bisphenol A

-  Bisphenol A
DTXSID7020182
-  Bisphenol A bis(2-hydroxyethyl ether) diacrylate
DTXSID6066991
-  Bisphenol A bis(2-hydroxyethyl ether) dimethacrylate
DTXSID1066992
-  Bisphenol A bis(2-hydroxypropyl) ether
DTXSID8051592
-  Bisphenol A carbonate polymer
DTXSID6027840
-  Bisphenol A diglycidyl ether
DTXSID6024624
-  Bisphenol A glycidyl methacrylate
DTXSID7044841
-  Bisphenol A propoxylate diglycidyl ether
DTXSID10399098
-  Bisphenol A propoxylate glycerolate diacrylate
DTXSID40400126

comptox-prod.epa.gov/dashboard

CompTox Dashboard Products and Use Categories



762 Thousand Chemicals



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

hair color

- CPDat PRODUCT category: personal care hair color
hair colors and dyes characterized as permanent
- CPDat PRODUCT category: personal care hair color
hair colors and dyes characterized as for professional use
- CPDat PRODUCT category: personal care hair color
hair colors and dyes characterized as temporary
- CPDat PRODUCT category: personal care hair color
hair coloring products not otherwise categorized
- CPDat PRODUCT category: personal care hair color activator
chemical activators for hair coloring products
- CPDat PRODUCT category: personal care hair color developer
chemical developers for hair coloring products
- CPDat PRODUCT category: personal care hair color toner
chemical toners for hair coloring products



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CompTox Dashboard Assays and Genes



762 Thousand Chemicals



Chemicals Product/Use Categories Assay/Gene

estrogen

- GENE: ESR1
estrogen receptor 1
- GENE: ESR2
estrogen receptor 2 (ER beta)
- GENE: ESRR A
estrogen-related receptor alpha
- GENE: ESRR B
estrogen-related receptor beta
- GENE: ESRR G
estrogen-related receptor gamma

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



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DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

▶ LITERATURE

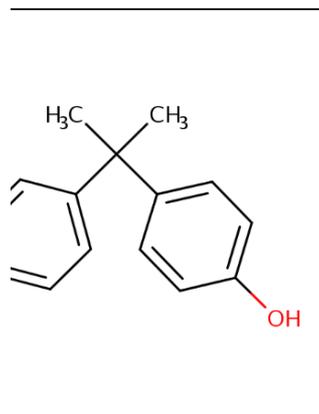
LINKS

COMMENTS

Bisphenol A

DTXSID7020182

US Tox Substance Id.



Batch Search Lists Predictions Downloads

Copy

Share

Submit Comment

Search all data

Wikipedia

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

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

...
[Read more](#)

Intrinsic Properties

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Quality Control Notes

Physicochemical properties

Property

Summary

Summary

LogP: Octanol-Water

Melting Point

Boiling Point

Water Solubility

Vapor Pressure

Flash Point

Surface Tension

Index of Refraction

Molar Refractivity

Polarizability

Density

Molar Volume

Thermal Conductivity

Viscosity

Henry's Law

LogKoa: Octanol-Air

Summary

Average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
		3.43	3.32	2.40 to 3.64	
	156	138	153 to 156	125 to 157	°C
		360	200	343 to 401	°C
		1.00e-3	5.26e-4	5.44e-4 to 1.31e-3	mol/L
		3.43e-7	-	6.83e-8 to 2.59e-6	mmHg
		190	-	188 to 192	°C
			-	46.0	dyn/cm
			-	1.60	
			-	68.2	cm ³
			-	27.0	Å ³
		1.17	-	1.14 to 1.20	g/cm ³
			-	200	cm ³
			-	150	mW/(m ² K)

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

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

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

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

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

 Journal of Cheminformatics

To link to th

RESEARCH ARTICLE

Open Access



OPERA models for predicting physicochemical properties and environmental fate endpoints

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

Detailed OPERA Prediction Reports

[Source](#)
[Result](#)
[Calculation Details](#)

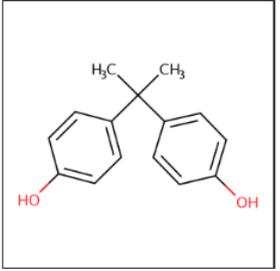
Experimental Values

- PhysPropNCCT
- Predicted Values
- EPISUITE
- NICEATM
- ACD/Labs Conse
- ACD/Labs
- OPERA

OPERA Models: LogP: Octanol-Water

[Save PDF](#)

Bisphenol A
80-05-7 | DTXSID7020182



Model Results

Predicted value: 3.35

Global applicability domain: inside

Local applicability domain index: 0.88

Confidence level: 0.75

Model Performance

Weighted KNN model

[QMR](#)

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.89	0.86	0.87	0.88	0.78

Nearest Neighbors from the Training Set

Bisphenol A
Measured: 3.32
Predicted: 3.35

BUTANOIC ACID,2-(4-BIPHENYL)-3-HYDROXY...
Measured: 3.25
Predicted: 3.45

Flurbiprofen
Measured: 4.18
Predicted: 3.83

2,2-Diphenylpropionic acid
Measured: 2.89
Predicted: 2.93

3-OH-2-(4-BIPHENYL)HEXANOIC ACID
Measured: 3.75
Predicted: 3.88

Access to Chemical Hazard Data

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

Data Type

Point of Departure ▼
 Download ▼

Human Eco

Columns 10

Search query

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

- ToxVal Database contains following data:
 - 30,050 chemicals
 - 772,721 toxicity values
 - 29 sources of data
 - 21,507 sub-sources
 - 4585 journals cited
 - 69,833 literature citations

In Vitro Bioassay Screening

ToxCast and Tox21

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

TOXCAST SUMMARY

PUBCHEM

TOXCAST DATA

TOXCAST MODELS

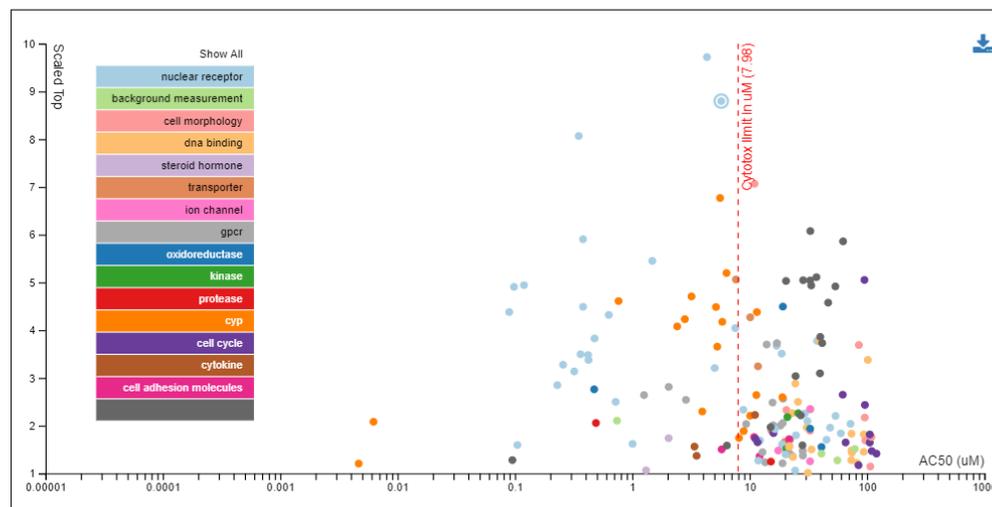
SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

Chemical Activity Summary i

TOXCAST DATA



ASSAY DETAILS

AC50 (uM): 5.73
Scaled top: 8.80
Assay Endpoint Name: OT_ER_ERaEa_0480
Assay Description: 742
Gene Symbol: ESR1
Organism: human
Tissue: kidney
Assay Format Type: cell-based
Biological Process Target: protein stabilization
Detection Technology: Protein-fragment Complementation
Analysis Direction: positive
Intended Target Family: nuclear receptor
Description: Data from the assay component OT_ER_ERaEa_0480 was analyzed into 1 assay endpoint. This assay endpoint, OT_ER_ERaEa_0480, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of binding reporter, measures of receptor for gain-of-signal activity can be used to understand the binding at the pathway-level as they relate to the gene ESR1. Furthermore, this assay endpoint can be referred to as a primary readout, because the performed assay has only produced 1 assay endpoint. To generalize the intended target to other relateable targets, this assay endpoint is annotated to the 'nuclear receptor' intended target family, where the subfamily is 'steroidal'.

In Vitro Bioassay Screening

ToxCast and Tox21

- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS

Download

Columns 10

Search query

Show Inactive Show Background

Name	Modal	Description	SeqPASS	Gene Name	AOP	Event	Hit Call	Top	Scaled Top	AC50	logAC50	Intended Target Family
ACEA_T47D_80hr_Negative		-	-	-	-	-	ACTIVE	35.5	1.65	65.8	1.82	cell cycle
ACEA_T47D_80hr_Positive		2	NP_000116.2	ESR1	200	1181	ACTIVE	109	4.49	0.381	-0.419	nuclear receptor
APR_HepG2_CellLoss_24h_dn		-	-	-	-	-	ACTIVE	1.20	1.81	106	2.02	cell cycle
APR_HepG2_MitoMass_24h_dn		-	-	-	-	-	ACTIVE	0.874	1.76	109	2.04	cell morphology
APR_HepG2_MitoMembPot_24h_dn		-	-	-	-	-	ACTIVE	5.92	7.07	11.0	1.04	cell morphology
APR_HepG2_OxidativeStress_24h_up		-	-	-	-	-	ACTIVE	1.20	1.47	110	2.04	cell cycle
APR_HepG2_CellLoss_72h_dn		-	-	-	-	-	ACTIVE	4.49	5.05	95.2	1.98	cell cycle
APR_HepG2_MitoMembPot_72h_dn		-	-	-	-	-	ACTIVE	2.71	3.69	85.3	1.93	cell morphology
APR_HepG2_MitoticArrest_72h_up		-	-	-	-	-	ACTIVE	1.66	1.17	84.7	1.93	cell cycle
APR_HepG2_OxidativeStress_72h_up		-	-	-	-	-	ACTIVE	1.80	1.65	106	2.02	cell cycle

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

Showing 1 to 10 of 161 records

In Vitro Bioassay Screening

ToxCast and Tox21

PROPERTIES

- ENV. FATE/TRANSPORT
- HAZARD
- ▶ ADME
- ▶ EXPOSURE
- ▼ **BIOACTIVITY**
- TOXCAST: SUMMARY
- PUBCHEM
- TOXCAST: DATA**
- TOXCAST: MODELS
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- ▶ LITERATURE
- LINKS
- COMMENTS

Assay Selection 1 Selected

Active Inactive All

Filter

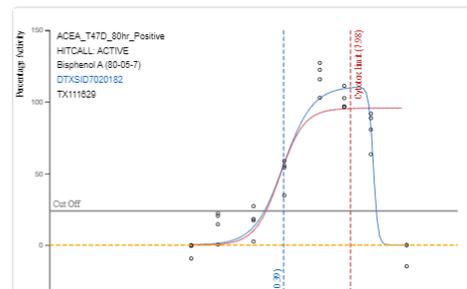
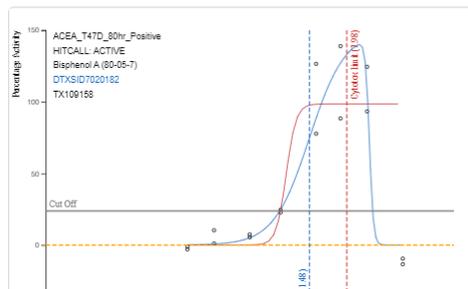
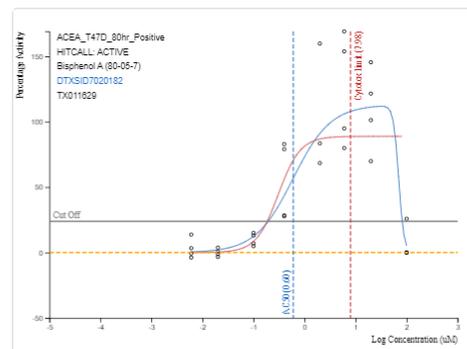
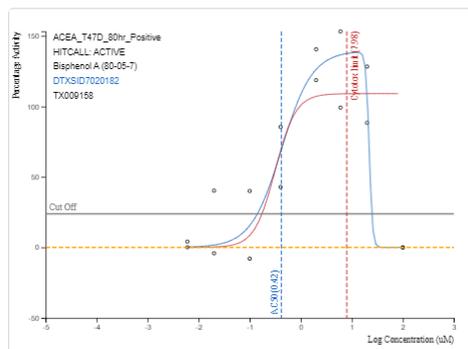
Filter assays

Assay Set: ER (1 of 18 Selected)

- ACEA_T47D_80hr_Positive**
- ATG_ERE_CIS_up**
- ATG_ERa_TRANS_up**
- NVS_NR_bER**
- NVS_NR_hER**
- NVS_NR_mERa**
- OT_ER_ERaERa_0480**
- OT_ER_ERaERa_1440**
- OT_ER_ERaERb_0480**
- OT_ER_ERaERb_1440**
- OT_ER_ERbERb_0480**
- OT_ER_ERbERb_1440**
- OT_ERa_EREGFP_0120**
- OT_ERa_EREGFP_0480**

A Single Assay Can Have Multiple Charts

Number of Charts: 6



Sources of Exposure to Chemicals

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

PRODUCT & USE CATEGORIES

CHEMICAL WEIGHT FRACTION

CHEMICAL FUNCTIONAL USE

TOXICS RELEASE INVENTORY

MONITORING DATA

EXPOSURE PREDICTIONS

PRODUCTION VOLUME

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Columns 10

Search query

Product and Use Categories (PUCs) i

Product or Use Categorization	Categorization type	Number of Unique Products
manufacturing, metals	CPCat Cassette	17
adhesive	CPCat Cassette	17
	CPCat Cassette	16
	CPCat Cassette	12
	CPCat Cassette	11
	CPCat Cassette	8
	CPCat Cassette	8
	CPCat Cassette	8
	CPCat Cassette	7
	CPCat Cassette	6

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

Bisphenol A

80-05-7 | DTXSID7020182

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DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

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TOXICS RELEASE INVENTORY

MONITORING DATA

EXPOSURE PREDICTIONS

PRODUCTION VOLUME

BIOACTIVITY

Toxics Release Inventory

Print Page

2015 TRI Factsheet: Chemical - 4,4'-ISOPROPYLIDENEDIPHENOL, 000080057

Data Source: 2016 Dataset (released March 2018)

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 4,4'-ISOPROPYLIDENEDIPHENOL



Quick Facts for 2015

	Chemical	United States
Number of TRI Facilities:	120	22,130
Total Production-Related Waste Managed:	15.8 million lbs	27.1 billion lbs
Total On-site and Off-site Disposal or Other Releases:	2.5 million lbs	3.4 billion lbs
Total On-site:	39.4 thousand lbs	2.9 billion lbs
• Air:	28.7 thousand lbs	686.4 million lbs
• Water:	4.4 thousand lbs	198.2 million lbs
• Land:	6.2 thousand lbs	2.0 billion lbs

Identifiers to Support Searches

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

25

Search query

Synonym

Quality

Bisphenol A

Valid

4,4'-(Propane-2,2-diyldiphenol

Valid

Phenol, 4,4'-(1-methylethylidene)bis-

Valid

80-05-7 Active CAS-RM

Valid

BPA

Valid

4,4'-Propane-2,2-diyldiphenol

Valid

Phenol, 4,4'-(1-methylethylidene)bis-

Valid

4-06-00-06717 Belstein Registry Number

Belstein

(4,4'-Dihydroxydiphenyl)dimethylmethane

Good

2,2-Bis(4'-hydroxyphenyl)propane

Good

2,2'-Bis(4-hydroxyphenyl)propane

Good

2,2-BIS-(4-HYDROXY-PHENYL)-PROPANE

Good

2,2-Bis(4-hydroxyphenyl)propane

Good

2,2-Bis(p-hydroxyphenyl)propane

Good

2,2-Di(4-Hydroxyphenyl) Propane

Good

Literature Searches and Links

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

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

Select a Query Term

Retrieve Articles

Select a Query Term

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

Optionally, edit the query before retrieving.

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

LITERATURE

GOOGLE SCHOLAR

PUBMED ABSTRACT SIFTER

PUBCHEM ARTICLES

PUBCHEM PATENTS

PPRTV

IRIS

Abstract Sifter – PubMed Integration

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

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SYNONYMS

▼ LITERATURE

GOOGLE SCHOLAR

PUBMED ABSTRACT SIFTER

PUBCHEM ARTICLES

PUBCHEM PATENTS

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

Hazard

Retrieve Articles

118 of 118 articles loaded...

Optionally, edit the query before retrieving.

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

Download / Send to...

Download Sifter for Excel

To find articles quickly, enter terms to sift abstracts.

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



SOFTWARE TOOL ARTICLE

Abstract Sifter: a comprehensive front-end system to PubMed [version 1; referees: 2 approved]

 Nancy Baker ¹, Thomas Knudsen², Antony Williams ²

 [Author details](#)



This article is included in the [Chemical Information Science](#) gateway.

Abstract

The Abstract Sifter is a Microsoft Excel based application that enhances existing search capabilities of PubMed. The Abstract Sifter assists researchers to search effectively, triage results, and keep track of articles of interest. The tool implements an innovative "sifter" functionality for relevance ranking, giving the researcher a way to find articles of interest quickly. The tool also gives



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629

 VIEWS

118

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External Links to ~80 websites

Bisphenol A

80-05-7 | DTXSID7020182
Searched by Approved Name.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ▶ ADME
- ▶ EXPOSURE
- ▶ 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
-  Chempid
-  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
-  ECHA Infocard
-  ChemAgora

Toxicology



Analytical

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

Prediction

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

Integrated Linkouts

eChemPortal provides free public access to information on properties of chemicals. Direct links to collections of chemical hazard and risk information prepared for government chemical review programmes at national, regional and international levels are obtained.



The International Chemical Safety Cards (ICSC) summarize essential health and safety information on chemicals for their use at the

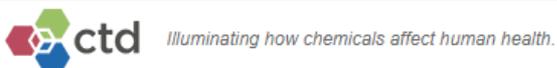
[NIOSH Chemical Safety ...](#)

Comparative Toxicogenomics Database is a robust, publicly available database that aims to advance understanding about how environmental exposures affect human health.



Integrated Linkouts

Comparative Toxicogenomics DB



YOUR QUERIES | CONTACT US

Chemicals

Comparative Toxicogenomics Database

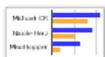
- Home
- Search
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Propylene Glycol

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

These diseases are associated with *Propylene Glycol* or its descendants. Each association is *curated* (**M** marker/mechanism and/or **T** therapeutic) and/or *inferred* (via a curated gene interaction).

Disease categories [\[Show chart\]](#)



Filter by Disease category: Association type:

1-50 of 240 results.

- First
- Previous
- 1
- 2
- 3
- 4
- 5
- Next
- Last

	Chemical	Disease	Direct Evidence	Enrichment Analysis	Inference Network	Inference Score	References
1.	Propylene Glycol	Drug-Related Side Effects and Adverse Reactions	M		2 genes: ABCC2 ABCC4	4.09	5
2.	Propylene Glycol	Acute Kidney Injury	M		2 genes: IL6 TGFB1	3.78	3
3.	Propylene Glycol	Chemical and Drug Induced Liver Injury	M		2 genes: ABCC2 IL6	2.82	5
4.	Propylene Glycol	Kidney Diseases	M		1 gene: TGFB1	2.54	4

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

(C10-C16) Alkylbenzenesulfonic acid

68584-22-5 | DTXSID2028723

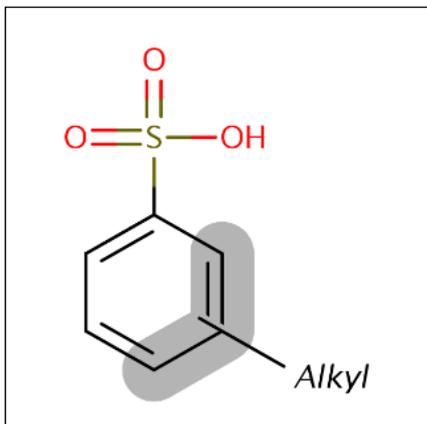
Searched by DSSTox Substance Id.

DETAILS

RELATED SUBSTANCES

PROPERTIES

COMMENTS



Intrinsic Properties

Presence in Lists

Federal

Safer Choice Chemical List TOX21SL: Tox21 Screening Library TSCA Workplan Step 2 Chemicals

EPAHFR - EPA Chemicals associated with hydraulic fracturing

US State

None.

International

OLEM RapidTox Chemicals REACH Dossier Chemicals

Other

Surfactant List Screened in Swiss Wastewater (2014) EDSP Universe TSCAACTIVE

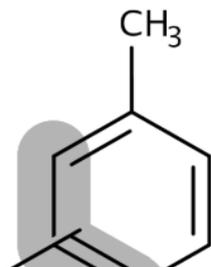
EPA Chemicals associated with hydraulic fracturing

Markush Structures

Xylenes

1330-20-7 | DTXSID2021446

Searched by DSSTox Substance Id.



Wikipedia

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

...
[Read more](#)

Intrinsic Properties

Presence in Lists

Record Information

DETAILS

RELATED SUBSTANCES

PROPERTIES

COMMENTS

8 chemicals

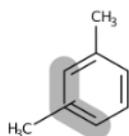
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Show info: DTXSID CASRN Select all

Sort by: Relationship

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Searched Chemical



Xylenes
DTXSID: DTXSID2021446
CASRN: 1330-20-7

Predecessor: Component

4 related chemical
structures with this
substance

Xylenes: defined mixture 1
DTXSID: DTXSID0021421
CASRN: NOCAS_21421

Predecessor: Component

4 related chemical
structures with this
substance

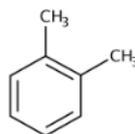
Xylenes: defined mixture 2
DTXSID: DTXSID7021447
CASRN: NOCAS_21447

Predecessor: Component

5 related chemical
structures with this
substance

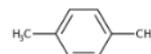
Total Petroleum Hydrocarbons (TPH)
DTXSID: DTXSID30801529
CASRN: NOCAS_091529

Markush Child



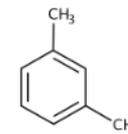
o-Xylene
DTXSID: DTXSID3021807
CASRN: 95-47-6

Markush Child



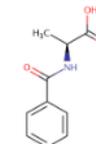
p-Xylene
DTXSID: DTXSID2021868
CASRN: 106-42-3

Markush Child



m-Xylene
DTXSID: DTXSID6026298
CASRN: 108-38-3

Transformation Product



N-Benzoylalanine
DTXSID: DTXSID40176394
CASRN: 2198-84-3

Chlorothalonil

1897-45-6 | DTXSID0020319

Searched by DSSTox Substance Id.

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

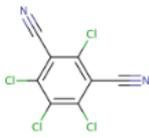
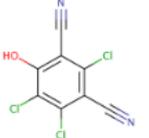
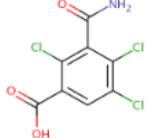
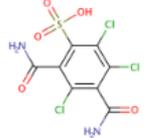
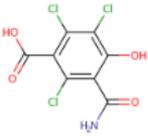
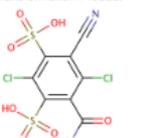
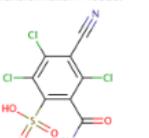
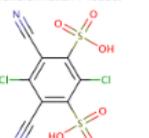
8 chemicals

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Searched Chemical	Transformation Product	Transformation Product	Transformation Product	Transformation Product
 <p>Chlorothalonil DTXSID: DTXSID0020319 CASRN: 1897-45-6</p>	 <p>4-Hydroxy-2,5,6-trichloroisophthalonitrile DTXSID: DTXSID0182588 CASRN: 28343-81-6</p>	 <p>3-Carbamoyl-2,4,5-trichlorobenzoic acid DTXSID: DTXSID10597537 CASRN: 142733-37-7</p>	 <p>2,4-dicarbamoyl-3,5,6-trichlorobenzene DTXSID: DTXSID30891327 CASRN: NOCAS_891327</p>	 <p>3-carbamoyl-2,5,6-trichloro-4-hydroxybenzoic acid DTXSID: DTXSID90891328 CASRN: NOCAS_891328</p>
	 <p>4-carbamoyl-2,5-dichloro-6-cyanobenzamide DTXSID: DTXSID00891329 CASRN: NOCAS_891329</p>	 <p>2-carbamoyl-3,5,6-trichloro-4-cyanobenzamide DTXSID: DTXSID00891330 CASRN: NOCAS_891330</p>	 <p>2,5-dichloro-4,6-dicyanobenzene-1,3-diamine DTXSID: DTXSID20891331 CASRN: NOCAS_891331</p>	

Not just chemical “structures”

- Different chemical substances supported
 - Chemical structures
 - “UVCB chemicals” - Unknown or Variable Composition, Complex Reaction Products and Biological Materials
 - Metabolites and transformation products
 - Homologous series as Markush Structures
 - Curated classes of chemicals
- **Lists of chemicals**
 - Submitted lists of chemicals – Federal, State, International and other general lists
 - Growing lists to support specific projects – e.g. ToxCast phases, algal toxins, our publication datasets

List of Chemicals

Lists of Chemicals

List of Assays

Select List

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

Algal Toxins

54 chemicals

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CASRN

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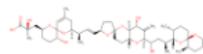
Sort by:

DTXSID



Filter by: Name or CASRN

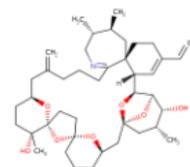
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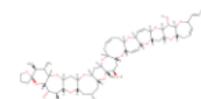
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CASRN: 81720-10-7



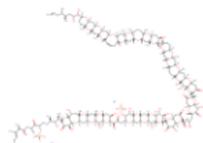
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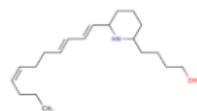
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CASRN: NOCAS_880102



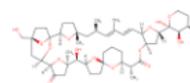
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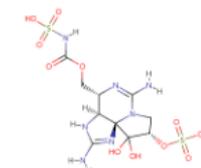
Maitotoxin
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CASRN: 59392-53-9



Euglenophycin
DTXSID: DTXSID10880017
CASRN: 1219817-69-2



Peclenotoxin-1
DTXSID: DTXSID10880092
CASRN: 97564-90-4



Gonyautoxin
DTXSID: DTXSID10880097
CASRN: 80226-62-6

Mass and Formula Searches Supporting Mass Spectrometry

Advanced Search

Mass Search

 ± Min/Max

Select Adduct: ▼

 Da

±

 Da ppm

Search Q

Molecular Formula Search

MS Ready Formula 

Exact Formula 

Search Q

Generate Molecular Formula(e)

 ± Min/Max Da

±

 Da ppm

Search Q

Default Options: C[1-50] H[0-100] O[0-20] N[0-20] P[0-20] S[0-10]

Include Halogens: F[0-20] Cl[0-20] Br[0-20] I[0-20]

Advanced Searches

Mass Based Search

Mass Search

Da

Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

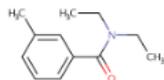
298 of 298 chemicals visible

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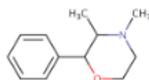
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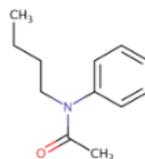
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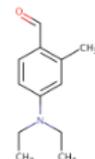
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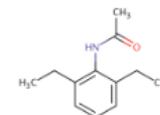
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CASRN: 634-03-7
TOXCAST: 0
Mass Diff: 0.000014



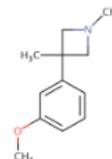
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Mass Diff: 0.000014



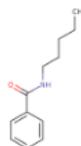
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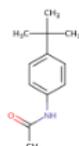
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CASRN: 16665-89-7
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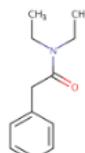
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CASRN: 19832-26-9
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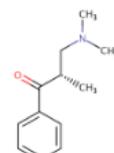
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CASRN: 20308-43-4



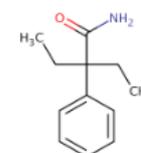
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CASRN: 20330-45-4



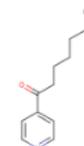
N,N-Diethylphenylacetamide
DTXSID: DTXSID00179048
CASRN: 2431-98-1



3-(Dimethylamino)-2-methylpropiofenone
DTXSID: DTXSID80180796
CASRN: 26171-60-6



Butyramide, 2-ethyl-2-phenyl-
DTXSID: DTXSID60184653
CASRN: 30568-39-0



1-Heptanone, 1-(4-pyridyl)-
DTXSID: DTXSID40188594
CASRN: 32941-30-3

Advanced Searches

Mass Based Search

Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

298 of 298 chemicals visible

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Select all

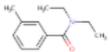
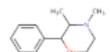
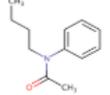
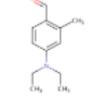
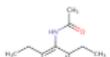


Sort by: Mass Difference



Filter by: Name or CASRN

Multicomponent Chemicals

Structure	DTXSID	Preferred Name	CASRN	QC Level	CPDat Count	Number of Sources	PubChem Data Sources	PubMed Ref. Counts	Monoisotopic Mass	Mass Difference
	DTXSID2021995 <small>ToxCast™</small>	DEET	134-82-3	Level 1	111	111	155	753	191.131014	0.000014
	DTXSID1023447	Phendimetrazine	634-03-7	Level 2	12	28	35	50	191.131014	0.000014
	DTXSID2042197	N-Butylacetanilide	91-49-6	Level 2	1	26	50	1	191.131014	0.000014
	DTXSID4059041	Benzaldehyde, 4-(diethylamino)-2-methyl-	92-14-8	Level 3	0	7	51	0	191.131014	0.000014
	DTXSID90168148	Acetanilide, 2,6'-diethyl-	16665-89-7	Level 4	0	4	33	0	191.131014	0.000014

- Singleton searches are useful but we work with thousands of chemicals!
- Typical questions
 - What are the SMILES strings for a list of 1000 chemicals?
 - Do any of this list of chemicals have XXX type of data?
 - What are the predicted logP values for a list of chemicals?
 - Can I get chemical lists in Excel files? In SDF files?

Batch Searching

Batch Search



Step Three: Select Download Data or Display Chemicals

Please enter one identifier per line 

Select Input Type(s)

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

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

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

Chemical Data

Batch Searching

Select Output Format:

 Excel 

 Download

Customize Results

- Select All
- Select All in Lists

Chemical Identifiers

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

Structures

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

Intrinsic And Predicted Properties

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

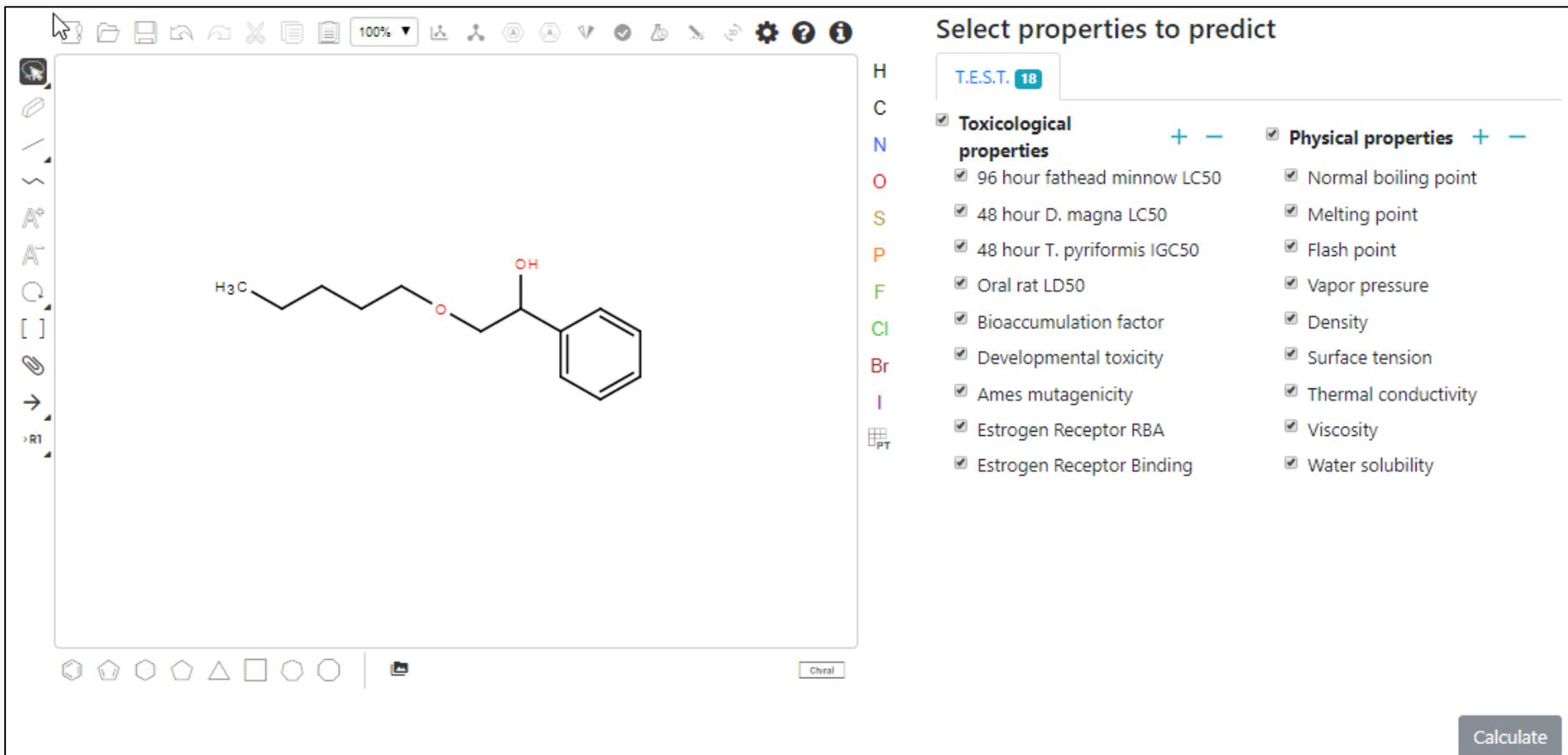
Presence in Lists:

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

Excel Output

INPUT	FOUND_BY	DTXCID_IN	DATA_SQ	TOXVAL_D	TOXCAST	TOXCAST	NUMBER_C	PUBCHEM	STO
C6H12O3	MS Ready	DTXCID701:	51	Y	0.36	2/562	24	83	Y
C6H12O3	MS Ready	DTXCID003:	67	Y	0.36	1/276	376	80	Y
C6H12O3	MS Ready	DTXCID106:	65	Y	4.42	5/113	6	77	Y
C6H12O3	MS Ready	DTXCID105:	45	Y	0.0	0/163	3	94	-
C6H12O3	MS Ready	DTXCID901:	38	Y	-	-	14	110	Y
C6H12O3	MS Ready	DTXCID402:	34	Y	0.0	0/113	-	53	Y
C6H12O3	MS Ready	DTXCID202:	31	Y	-	-	-	36	Y
C6H12O3	MS Ready	DTXCID202:	30	-	2.54	7/276	-	54	-
C6H12O3	MS Ready	DTXCID109:	26	Y	-	-	-	46	-
C6H12O3	MS Ready	DTXCID202:	24	Y	0.0	0/113	-	47	-
C6H12O3	MS Ready	DTXCID303:	22	Y	-	-	-	89	-
C6H12O3	MS Ready	DTXCID302:	20	Y	-	-	2	25	Y
C6H12O3	MS Ready	DTXCID407:	19	Y	-	-	12	62	-
C6H12O3	MS Ready	DTXCID704:	17	Y	-	-	-	64	-
C6H12O3	MS Ready	DTXCID704:	16	Y	-	-	3	49	-

Real-Time Predictions



Select properties to predict

T.E.S.T. 18

<input checked="" type="checkbox"/> Toxicological properties + -	<input checked="" type="checkbox"/> Physical properties + -
<input checked="" type="checkbox"/> 96 hour fathead minnow LC50	<input checked="" type="checkbox"/> Normal boiling point
<input checked="" type="checkbox"/> 48 hour D. magna LC50	<input checked="" type="checkbox"/> Melting point
<input checked="" type="checkbox"/> 48 hour T. pyriformis IGC50	<input checked="" type="checkbox"/> Flash point
<input checked="" type="checkbox"/> Oral rat LD50	<input checked="" type="checkbox"/> Vapor pressure
<input checked="" type="checkbox"/> Bioaccumulation factor	<input checked="" type="checkbox"/> Density
<input checked="" type="checkbox"/> Developmental toxicity	<input checked="" type="checkbox"/> Surface tension
<input checked="" type="checkbox"/> Ames mutagenicity	<input checked="" type="checkbox"/> Thermal conductivity
<input checked="" type="checkbox"/> Estrogen Receptor RBA	<input checked="" type="checkbox"/> Viscosity
<input checked="" type="checkbox"/> Estrogen Receptor Binding	<input checked="" type="checkbox"/> Water solubility

Calculate

Real-Time Predictions

Property	Experimental Value	Prediction				
		Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50		4.477 -Log10(mol/L) 6.954 mg/L	4.195 -Log10(mol/L) 13.288 mg/L	3.994 -Log10(mol/L) 21.110 mg/L	3.478 -Log10(mol/L) 69.224 mg/L	6.238 -Log10(mol/L) 0.120 mg/L
48 hour D. magna LC50		4.398 -Log10(mol/L) 8.328 mg/L	3.877 -Log10(mol/L) 27.677 mg/L	4.039 -Log10(mol/L) 19.026 mg/L	4.084 -Log10(mol/L) 17.173 mg/L	5.593 -Log10(mol/L) 0.532 mg/L
48 hour T. pyriformis IGC50		4.063 -Log10(mol/L) 18.039 mg/L	3.731 -Log10(mol/L) 38.668 mg/L		3.386 -Log10(mol/L) 85.610 mg/L	5.070 -Log10(mol/L) 1.773 mg/L
Oral rat LD50		1.758 -Log10(mol/kg) 3640.950 mg/kg	1.982 -Log10(mol/kg) 2172.756 mg/kg			1.533 -Log10(mol/kg) 6101.245 mg/kg
Bioaccumulation factor		1.797 Log10 62.700	2.202 Log10 159.310	1.287 Log10 19.346	1.181 Log10 15.157	2.520 Log10 330.834
Developmental toxicity		false	false	false		true
Ames mutagenicity		false	false			false
Estrogen Receptor RBA		-3.075 Log10 8.418*10 ⁻⁴	-3.078 Log10 8.356*10 ⁻⁴	-3.720 Log10 1.907*10 ⁻⁴		-2.427 Log10 0.004
Estrogen Receptor Binding		true	true	true	false	true

Our support for FAIR Data

F
Findable



A
Accessible



I
Interoperable



R
Reusable



Downloadable Data



DSSTox Identifier to PubChem Identifier Mapping File

Posted: 11/14/2016

The DSSTox to PubChem Identifiers mapping file is in TXT format and includes the PubChem SID, PubChem CID and DSSTox substance identifier (DTXSID).

SID	CID	DTXSID
316388891	20404	DTXSID30873143
316388890	10142816	DTXSID70873142
316388889	50742127	DTXSID40873139
316388888	19073841	DTXSID20873137
316388887	11505215	DTXSID00873135
316388886	25021861	DTXSID80873133
316388885	2784427	DTXSID60873131
316388884	6731	DTXSID00873130

DSSTox identifiers mapped to CAS Numbers and Names File

Posted: 11/14/2016

The DSSTox Identifiers file is in Excel format and includes the CAS Number, DSSTox substance identifier (DTXSID) and the Preferred Name.

1	casrn	dsstox_substance_id	preferred_name
2	26148-68-5	DTXSID7020001	A-alpha-C
3	107-29-9	DTXSID2020004	Acetaldehyde oxime
4	60-35-5	DTXSID7020005	Acetamide
5	103-90-2	DTXSID2020006	Acetaminophen
6	968-81-0	DTXSID7020007	Acetohexamide
7	18523-69-8	DTXSID2020008	Acetone[4-(5-nitro-2-furyl)-2-thiazolyl] hydrazone
8	75-05-8	DTXSID7020009	Acetonitrile
9	127-06-0	DTXSID6020010	Acetoxime
10	65734-38-5	DTXSID6020012	N'-Acetyl-4-(hydroxymethyl) phenylhydrazine

- Present work in development
 - Real time prediction using OPERA models
 - Structure/substructure/similarity search integration
 - Ongoing expansion of chemicals
 - Release of new ToxCast database (v3_2018)
 - Addition of products data from 10s of thousands of MSDS sheets
 - Analytical Data support
 - Integration of analytical data for ToxCast/Tox21 data
 - Spectral searching against predicted Mass Spectra

Prototype Development

AADashboard

atrazine

Search



Select properties to predict

H
C
N
O

T.E.S.T. 18 OPERA Search

Exact
 Substructure

Search result 2540

Show Isotopically Labeled Charged Salts or Mixtures

Sort Similarity

 1	 0.62	 0.57	 0.57	 0.57	 0.57	 0.53	 0.53	 0.53	 0.5	 0.5	 0.5
 0.5	 0.5	 0.5	 0.47	 0.44	 0.44	 0.44	 0.44	 0.42	 0.42	 0.42	 0.42
 0.42	 0.42	 0.42	 0.42	 0.42	 0.4						
 0.4											
 0.38											

Search result 2540

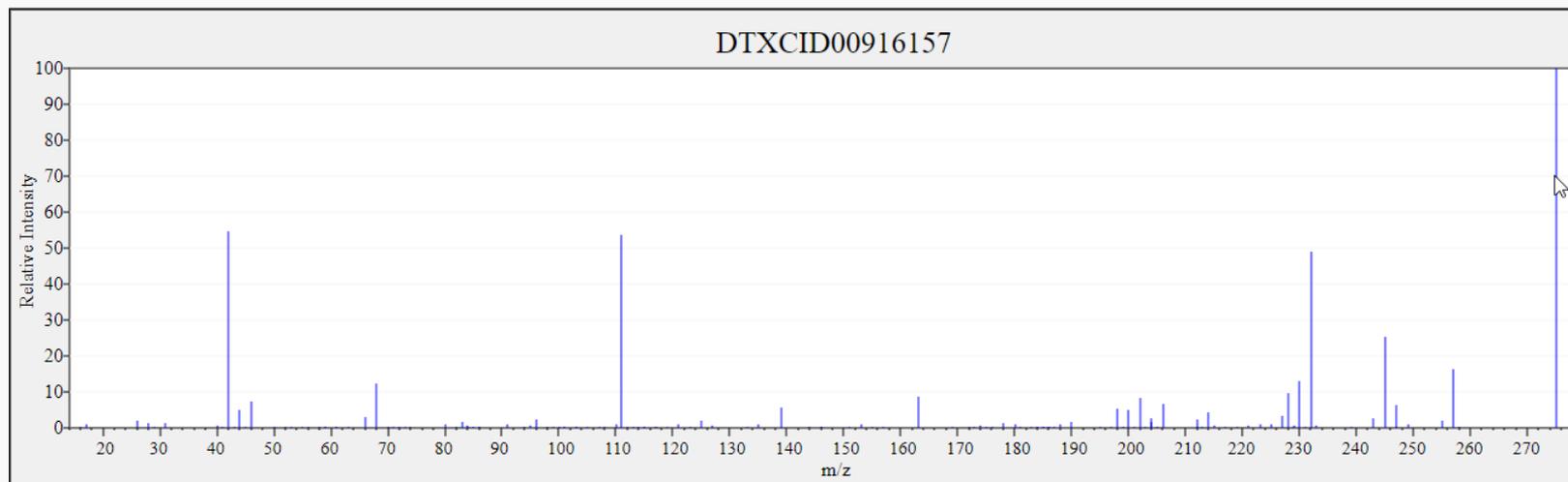
Show Isotopically Labeled

Predicted Mass Spectra

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



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



- The EPA CompTox Dashboard provides access to data for ~875,000 chemicals, ToxCast assays and associated product use categories
- High quality data from ongoing curation efforts
- An integration hub for multiple “modules”
 - Experimental and predicted properties
 - Human and Ecological Hazard data
 - Exposure data – products, data in the environment
 - *In vitro* bioassay data – ToxCast/Tox21
 - Literature searching – Google Scholar and PubMed
 - Specialized searches – mass/formula for analytical support
 - Batch searching and Real Time Predictions
- Data and functionality increases with every release

- The NCCT CompTox Chemistry Dashboard Development Team
- NERL scientists (Jon Sobus, Elin Ulrich) – Mass Spectrometry
- Kamel Mansouri – OPERA models
- Todd Martin and Valery Tkachenko – TEST predictions
- Nancy Baker – Abstract Sifter

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