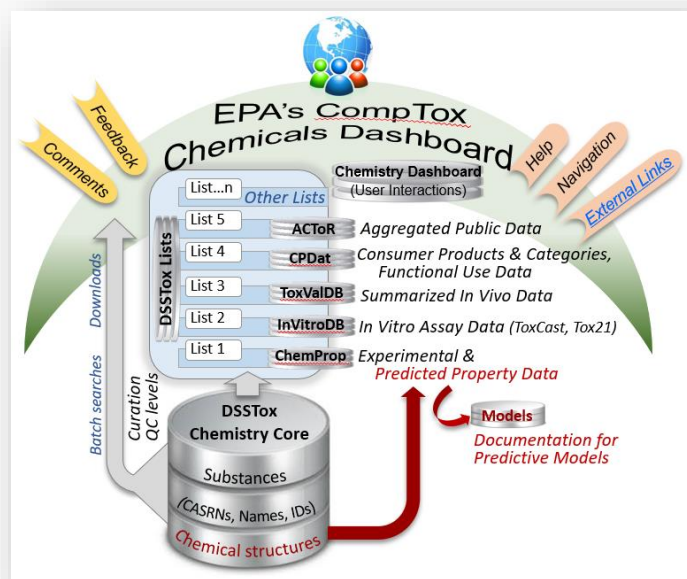


# EPA CompTox Chemicals Dashboard as a Data Integration Hub for Environmental Chemistry Data



*Antony Williams*

*Center for Computational Toxicology and Exposure,  
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*

*November 2019*

*Decontamination Conference, Norfolk, VA*

- Freely accessible website and integration hub
  - Chemical substances – the majority with structures
  - Searchable by chemical, product use and gene
  - Experimental and predicted physicochemical property data
  - Experimental and predicted fate and transport data
  - Bioactivity data for the ToxCast/Tox21 project
  - Literature searches for chemicals using public resources
  - Links to other agency websites and public data resources
  - Batch searching for *thousands* of chemicals
  - Chemical lists of interest – pesticides, leachables, PFAS



# A data integration hub

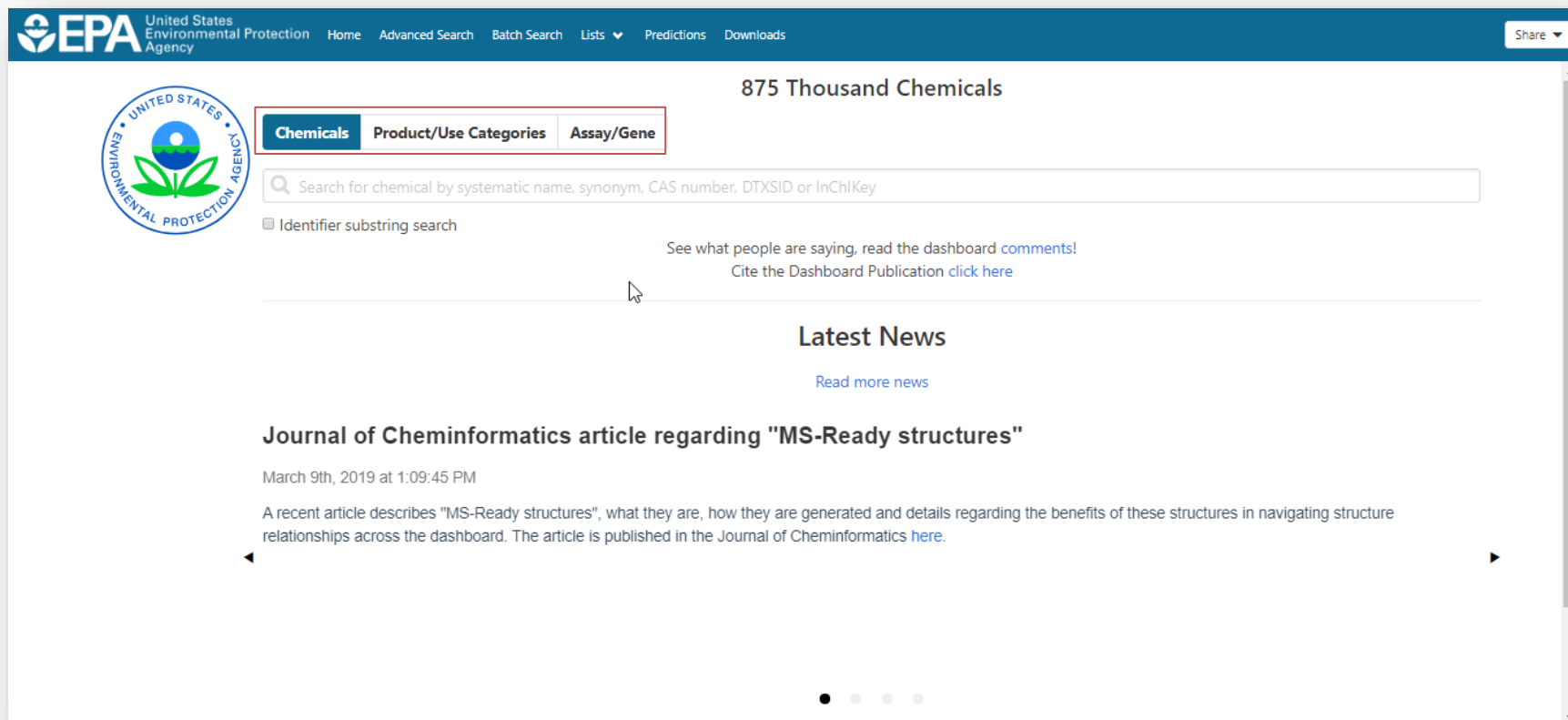
## LOTS of data!

- >875,000 chemicals curated over 20 years
- >700,000 toxicity data points from >30 sources
- Millions of synonyms and identifiers
- Tens of thousands of experimental data points
- Millions of QSAR prediction reports
- Millions of bioactivity data points for >4000 chemicals and hundreds of assay end points
- Searching of Pubmed's 29 million abstracts

# CompTox Chemicals Dashboard

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

## 875k Chemical Substances



The screenshot shows the EPA CompTox Chemicals Dashboard. The header features the EPA logo and navigation links: Home, Advanced Search, Batch Search, Lists, Predictions, and Downloads. A 'Share' button is in the top right. The main content area is titled '875 Thousand Chemicals'. It includes a search bar with the placeholder text 'Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey'. Below the search bar is a checkbox for 'Identifier substring search'. To the right of the search bar, there are links to 'See what people are saying, read the dashboard comments!' and 'Cite the Dashboard Publication click here'. The 'Latest News' section features an article titled 'Journal of Cheminformatics article regarding "MS-Ready structures"' dated March 9th, 2019 at 1:09:45 PM. The article text describes 'MS-Ready structures' and their benefits in navigating structure relationships. A 'Read more news' link is provided. The dashboard also includes a circular EPA logo on the left and a 'Chemicals' tab selected among 'Product/Use Categories' and 'Assay/Gene'.

United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share

875 Thousand Chemicals

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](#)

Latest News

[Read more news](#)


**Journal of Cheminformatics article regarding "MS-Ready structures"**


March 9th, 2019 at 1:09:45 PM

A recent article describes "MS-Ready structures", what they are, how they are generated and details regarding the benefits of these structures in navigating structure relationships across the dashboard. The article is published in the Journal of Cheminformatics [here](#).

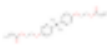
# BASIC Search

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

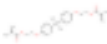
 Bisphenol



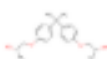
Bisphenol A  
DTXSID7020182



Bisphenol A bis(2-hydroxyethyl ether) diacrylate  
DTXSID6066991

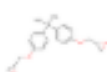


Bisphenol A bis(2-hydroxyethyl ether) dimethacrylate  
DTXSID1066992

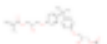


Bisphenol A bis(2-hydroxypropyl) ether  
DTXSID8051592

Bisphenol A carbonate polymer  
DTXSID6027840



Bisphenol A diglycidyl ether  
DTXSID6024624




Bisphenol A glycidyl methacrylate  
DTXSID7044841

# Detailed Chemical Pages

**EPA** United States  
Environmental Protection  
Agency

Home Advanced Search Batch Search Lists Predictions Downloads

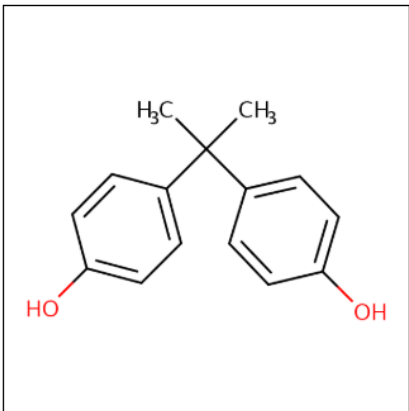
Copy Share Submit Comment Search all data



## 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**



# An "Executive Summary" Quick Look Tox Info

## Executive Summary

### Quantitative Risk Assessment Values

- ✓ IRIS values available [↗](#)
- ✗ No PPRTV values
- ✓ EPA RSL values available [↗](#)
- ✓ Minimum RfD: 0.050 mg/kg-day (chronic, IRIS, oral, 8) [↗](#)
- ✗ No RfC calculated
- ✗ IVIVE POD not calculated

### Quantitative Hazard Values

- ✓ Minimum oral POD: 3.8 mg/kg-day (reproductive, HPVIS, oral, 6) [↗](#)
- ✗ No inhalation POD values
- ✓ Lowest Observed Bioactivity Equivalent Level: CYP1A1, CYP1A2, Tpo, ESR2, ESR1, ESR1, NR1I3, PPARA, NR1I2, Cyp2c11, MMP3, Esr1

### Cancer Information

- ✗ No cancer slope factor
- ✗ No inhalation unit risk value
- ✓ Carcinogenicity data available: University of Maryland carcinogenicity warning: [↗](#)
- ✗ No genotoxicity findings reported

### Reproductive Toxicology

- ✓ 200 Reproductive toxicity PODs available [↗](#)

### Chronic Toxicology

- ✓ 340 Chronic toxicity PODs available [↗](#)

### Subchronic Toxicology

- ✓ 12 Subchronic toxicity PODs available [↗](#)

### Developmental Toxicology

- ✓ 6 Developmental toxicity PODs available [↗](#)

### Acute Toxicology

- ✓ 391 Acute toxicity PODs available [↗](#)

### Subacute Toxicology

- ✓ 1 subacute toxicity PODs available [↗](#)

### Neurotoxicology

- ✗ No neurotoxicology data available.

### Endocrine System

- ✓ Endocrine Disruption Potential. Significant Estrogen and Androgen Receptor activity seen. Chemical was positive in 21 ER assays (out of 35) and was positive in 9 AR assays (tested in 19).

### ADME

- ✓ HTTK C<sub>ss</sub> data are available [↗](#)

### Fate and Transport

- ✗ No bioaccumulation concern.
- ✗ No volatility concern.
- ✓ Biodegradation predictions are available [↗](#)
- ✓ BCF predictions are available [↗](#)
- ✓ Vapor Pressure predictions are available [↗](#)

### Exposure

- ✓ Exposure estimates are available based on NHANES and SEEM [↗](#)

### AOP Information

- ✓ AOP Links: 13, 33, 36, 58, 60, 61, 66, 107, 124, 150, 163, 175, 187, 200

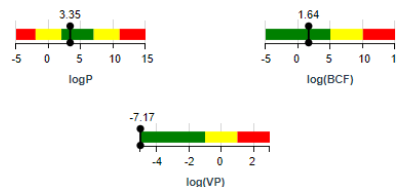
### Other Notes

- ✗ No water quality values available.
- ✗ No air quality values available.
- ✓ 14 Occupational exposure values available. [↗](#)

## REGIONAL SCREENING

Class	THQ	Value
risk-based SSL (mg/kg)	THQ = 0.1	5.8
GIABS (unspecified)	THQ = 1	1
GIABS (unspecified)	THQ = 0.1	1
ABS (unspecified)	THQ = 0.1	0.1
RfDo (mg/kg-day)	THQ = 0.1	0.05
screening level (residential soil) (mg/kg)	THQ = 0.1	320
screening level (industrial soil) (mg/kg)	THQ = 0.1	4100
screening level (tap water) (ug/L)	THQ = 0.1	77
RfDo (mg/kg-day)	THQ = 1	0.05
screening level (residential soil) (mg/kg)	THQ = 1	3200
screening level (industrial soil) (mg/kg)	THQ = 1	41000
ABS (unspecified)	THQ = 1	0.1
risk-based SSL (mg/kg)	THQ = 1	58
screening level (tap water) (ug/L)	THQ = 1	770

## PHYSICHEM PARAMETERS



## Quantitative Risk Assessment Values

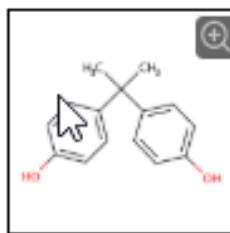
- ✓ IRIS values available [↗](#)
- ✗ No PPRTV values
- ✓ EPA RSL values available [↗](#)
- ✓ Minimum RfD: 0.050 mg/kg-day (chronic, IRIS, oral, 8) [↗](#)
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## Quantitative Hazard Values

- ✓ Minimum oral POD: 3.8 mg/kg-day (reproductive, HPVIS, oral, 6) [↗](#)
- ✗ No inhalation POD values
- ✓ Lowest Observed Bioactivity Equivalent Level: CYP1A1, CYP1A2, Tpo, NR1I3, PPARA, NR1I2, Cyp2c11, MMP3, Esr1



# Experimental and Predicted Data



**Bisphenol A**

**80-05-7 | DTXSID7020182**

Searched by DSSTox Substance Id.

Property



Summary



Download



Columns



Property	Experimental average	Predicted average	
<a href="#">LogP: Octanol-Water</a>	3.32 (1)	3.29	
<a href="#">Melting Point</a>	155 (7)	139	
<a href="#">Boiling Point</a>	200 (1)	363	
<a href="#">Water Solubility</a>	5.26e-4 (1)	9.62e-4	
<a href="#">Vapor Pressure</a>	-	8.37e-7	
<a href="#">Flash Point</a>	-	190	

# Transparency for prediction models

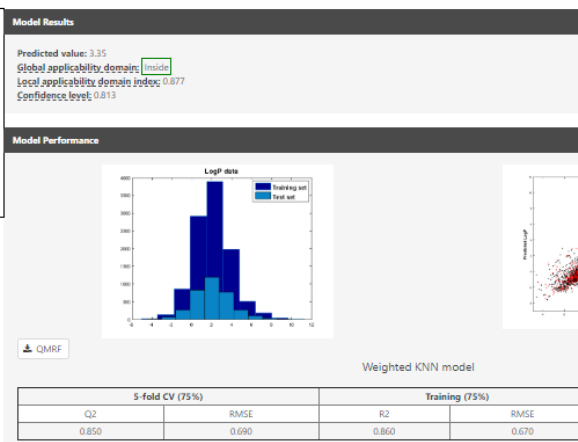
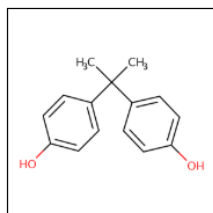
## Predicted

Download Predicted Data

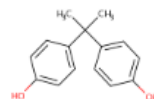
Source	Result	Calculation Details	QMRF
<a href="#">EPISUITE</a>	3.64	Not Available	Not Available
<a href="#">NICEATM</a>	2.40	Not Available	<a href="#">Available</a>
<a href="#">ACD/Labs Consensus</a>	3.63	Not Available	Not Available
<a href="#">ACD/Labs</a>	3.43	Not Available	Not Available
<a href="#">OPERA</a>	3.35	<a href="#">OPERA Model Report [Inside AD]</a>	<a href="#">Available</a>

## OPERA Models: LogP: Octanol-Water

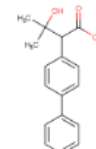
Bisphenol A  
80-05-7 | DTXSID7020182



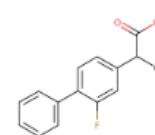
## Nearest Neighbors from the Training Set



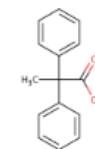
Bisphenol A  
Measured: 3.32  
Predicted: 3.35076



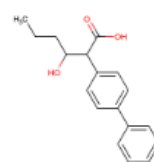
BUTANOIC ACID 2-(4-BIPHENYL)-3-HYDROXY-3-METHYL-  
Measured: 3.25  
Predicted: 3.39062



Flurbiprofen  
Measured: 4.16  
Predicted: 3.94445

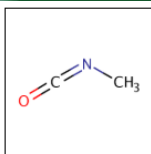


2,2-Diphenyldecanoic acid  
Measured: 2.69  
Predicted: 2.84603



3-OH-2-(4-BIPHENYL)-HEXANOIC ACID  
Measured: 3.75  
Predicted: 3.70322

# Access to Chemical Hazard Data



## Methyl isocyanate

624-83-9 | DTXSID1023786

Searched by DSSTox Substance Id.

### Hazard

DataType

 Toxicity Value 


















 Human  Eco

 Download 

Columns 

10 

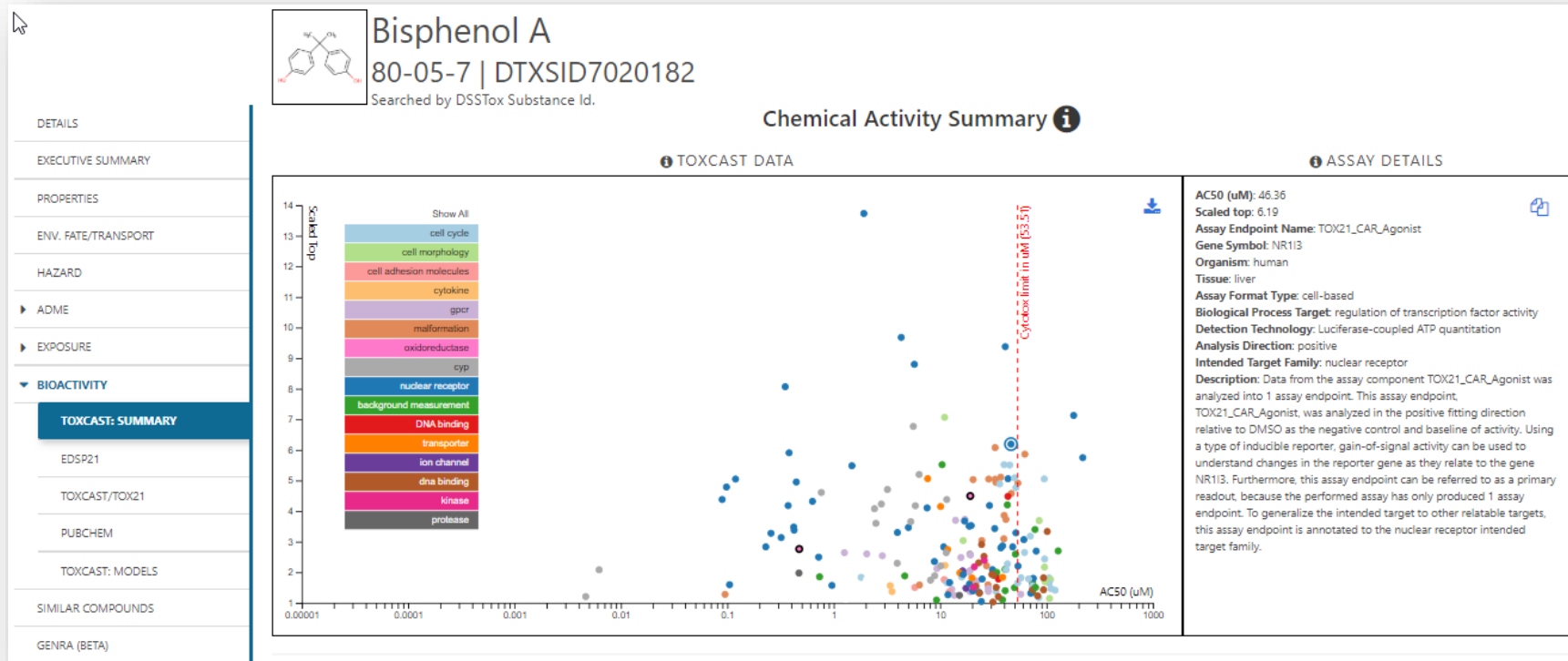
Search query

More 	Type 	Risk assessment class 	Value 	Units 	Exposure route 	Subsource 	Source 
	RfC	chronic	0.001	mg/m3	-	MSC Table 5	<a href="#">Pennsylvania DEP ToxValues</a>
	AEGL 2 - 8 hr (final)	acute	0.008	ppm	inhalation	EPA OW	<a href="#">EPA AEGL</a>
	MEG	short-term	0.016	mg/m3	inhalation	TG 230 Military Exposure Guidelines Table	<a href="#">DOD</a>
	MEG	chronic	0.016	mg/m3	inhalation	TG 230 Military Exposure Guidelines Table	<a href="#">DOD</a>
	AEGL 2 - 4 hr (final)	acute	0.017	ppm	inhalation	EPA OW	<a href="#">EPA AEGL</a>
	MEG	short-term	0.02	mg/m3	inhalation	TG 230 Military Exposure Guidelines Table	<a href="#">DOD</a>
	MEG	short-term	0.02	mg/m3	inhalation	TG 230 Military Exposure Guidelines Table	<a href="#">DOD</a>
	AEGL 3 - 8 hr (final)	acute	0.025	ppm	inhalation	EPA OW	<a href="#">EPA AEGL</a>
	AEGL 3 - 4 hr (final)	acute	0.05	ppm	inhalation	EPA OW	<a href="#">EPA AEGL</a>
	MEG	short-term	0.058	mg/m3	inhalation	TG 230 Military Exposure Guidelines Table	<a href="#">DOD</a>


- ToxVal Database contains following data:
  - ~800,000 toxicity values
  - ~30 sources of data
  - ~22,000 sub-sources
  - ~5000 journals cited
  - ~70,000 literature citations

# In Vitro Bioassay Screening

## ToxCast and Tox21



# Sources of Exposure to Chemicals

 **United States  
Environmental Protection  
Agency**

Home Advanced Search Batch Search Lists ▼ Predictions Downloads

Copy ▼ Share ▼ Submit Comment

## Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ ADME

Download ▼

Columns ▼ 10 ▼

### Product and Use Categories (PUCs)

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

▼ EXPOSURE

PRODUCT & USE CATEGORIES

CHEMICAL WEIGHT FRACTION

CHEMICAL FUNCTIONAL USE

TOXICS RELEASE INVENTORY

MONITORING DATA

EXPOSURE PREDICTIONS

PRODUCTION VOLUME

# Sources of Exposure to Chemicals

## Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

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ENV. FATE/TRANSPORT

HAZARD

► ADME

▼ EXPOSURE

PRODUCT & USE CATEGORIES

CHEMICAL WEIGHT FRACTION

CHEMICAL FUNCTIONAL USE

**TOXICS RELEASE INVENTORY**

MONITORING DATA

EXPOSURE PREDICTIONS

PRODUCTION VOLUME

▼ BIOACTIVITY

## Toxics Release Inventory

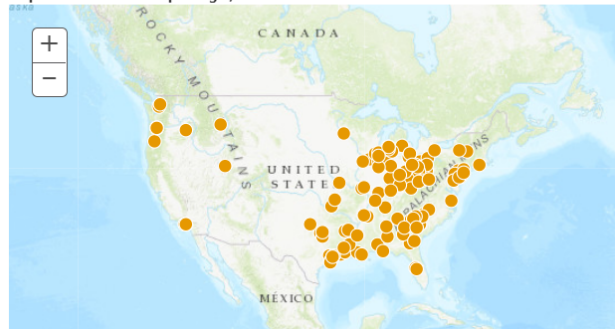
Print Page

### 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
<b>Number of TRI Facilities:</b>	120	22,130
<b>Total Production-Related Waste Managed:</b>	15.8 million lbs	27.1 billion lbs
<b><a href="#">Total On-site and Off-site Disposal or Other Releases:</a></b>	2.5 million lbs	3.4 billion lbs
<b><a href="#">Total On-site:</a></b>	39.4 thousand lbs	2.9 billion lbs
• <a href="#">Air:</a>	28.7 thousand lbs	686.4 million lbs
• <a href="#">Water:</a>	4.4 thousand lbs	198.2 million lbs
• <a href="#">Land:</a>	6.2 thousand lbs	2.0 billion lbs



# Identifiers to Support Searches



United States Environmental Protection Agency

HomeAdvanced SearchBatch SearchLists ▼PredictionsDownloads

Copy ▼Share ▼Submit Comment

Search all data

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

**SYNONYMS**

▶ LITERATURE

LINKS

COMMENTS

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

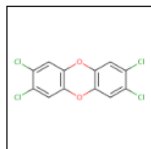
25 ▼

Search query

Synonym	Quality
Bisphenol A	Valid
4,4'-(Propane-2,2-diyl)diphenol	Valid
Phenol, 4,4'-(1-methylethylidene)bis-	Valid
80-05-7 <span>Active CAS-RN</span>	Valid
BPA	Valid
4,4'-Propane-2,2-diylidiphenol	Valid
Phenol, 4,4'-(1-methylethylidene)bis-	Valid
4-06-00-06717 <span>Beilstein Registry Number</span>	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

# What if we have nothing for you?

## “EXTERNAL LINKS”





















2,3,7,8-Tetrachlorodibenzo-p-dioxin



















1746-01-6 | DTXSID2021315

Searched by DSSTox Substance Id.


















### General

-  EPA Substance Registry Service
-  Household Products Database
-  PubChem
-  Chemspider
-  CPCat
-  DrugBank
-  Wikipedia
-  MSDS Lookup
-  ChEMBL
-  Chemical Vendors
-  ToxPlanet
-  ACS Reagent Chemicals
-  ChemHat: Hazards and Alternatives Toolbox
-  Wolfram Alpha
-  ECHA Infocard
-  ChemAgora
-  ChEBI
-  NIST Chemistry Webbook













### Toxicology

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





### Publications

-  Toxline
-  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

-  RSC Analytical Abstracts
-  Tox21 Analytical Data
-  MONA: MassBank North America
-  mzCloud
-  NIST NIST IR Spectrum
-  NIST NIST MS Spectrum
-  MassBank
-  NEMI: National Environmental Methods Index
-  NIST NIST Antoine Constants
-  IR Spectra on PubChem
-  NIST NIST Kovats Index values
-  Protein DataBank

### Prediction

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

# External Links



 PubChem Safety Sheet

 NIOSH Chemical Safety Cards



**Wireless Information System  
for Emergency Responders**

[WebWISER Home](#)

[Substance List](#)

[Help Identify](#)

[Tools](#)

[Help](#)

[Current Profile](#)

 1st Responder



[Key Info](#)

[Identification](#)

**[Protective Equipment /  
Clothing](#)**

[Fire Fighting Procedures](#)

[Reactivities / Incompatibilities](#)

[Treatment Overview](#)

- ▶ [Basic](#)
- ▶ [Properties](#)
- ▶ [Hazmat](#)
- ▶ [Medical](#)
- ▶ [Environment](#)

## 2,3,7,8-Tetrachlorodibenzo-p-dioxin

CAS RN: 1746-01-6

### Protective Equipment / Clothing

PRECAUTIONS FOR "CARCINOGENS": ... Dispensers of liq detergent /should be available./ ... Safety pipettes should be used for all pipetting. ... In animal laboratory, personnel should ... wear protective suits (preferably disposable, one-piece & close-fitting at ankles & wrists), gloves, hair covering & overshoes. ... In chemical laboratory, gloves & gowns should always be worn ... however, gloves should not be assumed to provide full protection. Carefully fitted masks or respirators may be necessary when working with particulates or gases, & disposable plastic aprons might provide addnl protection. ... Gowns ... /should be/ of distinctive color, this is a reminder that they are not to be worn outside the laboratory. /Chemical Carcinogens/

▶ [Handling Chemical Carcinogens in the Laboratory](#)

Wear appropriate personal protective clothing to prevent skin contact.

▶ [National Institute for Occupational Safety and Health](#)

Wear appropriate eye protection to prevent eye contact.

▶ [National Institute for Occupational Safety and Health](#)

Eyewash fountains should be provided in areas where there is any possibility that workers could be exposed to the substance; this is irrespective of the recommendation involving the wearing of eye protection.



 [PubChem Safety Sheet](#)

 [NIOSH Chemical Safety Cards](#)

[PUBCHEM](#) > [2,3,7,8-TETRACHLOROD...](#) > [GHS CLASSIFICATION](#)




CID 15625

# 2,3,7,8-Tetrachlorodibenzo-P-dioxin

## GHS Classification



Showing 3 of 3

Pictogram(s)	   Acute Toxic      Irritant      Environmental Hazard
Signal	<b><u>Danger</u></b>
GHS Hazard Statements	<p>Aggregated GHS information provided by 23 companies from 1 notifications to the ECHA C&amp;L Inventory. Each notification may be associated with multiple companies.</p> <p>H300 (100%): Fatal if swallowed [<b><u>Danger</u></b> Acute toxicity, oral]</p> <p>H319 (100%): Causes serious eye irritation [<b><u>Warning</u></b> Serious eye damage/eye irritation]</p> <p>H400 (100%): Very toxic to aquatic life [<b><u>Warning</u></b> Hazardous to the aquatic environment, acute hazard]</p> <p>H410 (100%): Very toxic to aquatic life with long lasting effects [<b><u>Warning</u></b> Hazardous to the aquatic environment, long-term hazard]</p> <p>Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.</p>

# External Links



 PubChem Safety Sheet

 NIOSH Chemical Safety Cards

[« back to the search result list](#)

English - EN ▼

## 2,3,7,8-TETRACHLORODIBENZO-p-DIOXIN

ICSC: 1467

Dibenzo [b,e] [1,4]dioxin, 2,3,7,8-tetrachloro-

2,3,7,8-TCDD

2,3,7,8-Tetrachloro-1,4-dioxin

November 2003

CAS #: 1746-01-6

UN #: 2811

EC Number: 217-122-7

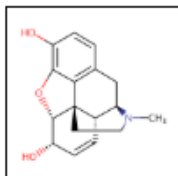
	ACUTE HAZARDS	PREVENTION	FIRE FIGHTING
FIRE & EXPLOSION	Gives off irritating or toxic fumes (or gases) in a fire.		In case of fire in the surroundings, use appropriate extinguishing media.

### AVOID ALL CONTACT! IN ALL CASES CONSULT A DOCTOR!

	SYMPTOMS	PREVENTION	FIRST AID
Inhalation	Symptoms may be delayed.	Use appropriate engineering controls.	Fresh air, rest. Refer for medical attention.
Skin	MAY BE ABSORBED! See Inhalation. Redness. Pain.	Protective gloves. Protective clothing.	Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer for medical attention .
Eyes	Redness. Pain.	Wear face shield or eye protection in combination with breathing protection.	First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.
Ingestion	See Inhalation.	Do not eat, drink, or smoke during work. Wash hands before eating.	Give a slurry of activated charcoal in water to drink. Induce vomiting (ONLY IN CONSCIOUS PERSONS!). Refer for medical attention .

SPILLAGE DISPOSAL	CLASSIFICATION & LABELLING
Evacuate danger area! Consult an expert! Personal protection: chemical protection suit including self-contained breathing apparatus.	According to UN GHS Criteria  Transportation UN Classification UN Hazard Class: 6.1; UN Pack Group: I
STORAGE	
Separated from food and feedstuffs.	
PACKAGING	

***Built in “Modules”***




## Morphine

57-27-2 | DTXSID9023336

Searched by Approved Name.

### Abstract Sifter

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
- Disaster / Emergency

Optionally, edit the query before retrieving.

"57-27-2" OR "Morphine"



# Literature Searching

Child (Infant through adolescent)

Dust and Exposure


Food and Exposure

Water and Exposure

Algae

Disaster / Emergency



 Optionally, edit the query before retrieving.

("57-27-2" OR "Morphine") AND ((water OR groundwater OR drinking water) AND Environmental Exposure)





# ***Chemical Lists***

# EPAHFR: Hydraulic Fracturing



## Select List

[Download](#) ▼[Columns](#) ▼[Copy Filtered Lists URL](#)

List Acronym ▼	List Name ▼	Last Updated ▼	Number of Chemicals ▼	List Description ▼
<a href="#">40CFR355</a>	<a href="#">40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities</a>	2018-01-05	354	Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378)
<a href="#">HAZSUBST</a>	<a href="#">WIKILIST: Extremely hazardous substances</a>	2018-11-23	336	The list of extremely hazardous substances is defined in Section 302 of the U.S. Emergency Planning and Community Right-to-Know Act (42 U.S.C. 11002)
<a href="#">NRTCHEMICALS</a>	<a href="#">US National Response Team Chemical Set</a>	2018-05-11	18	The U.S. National Response Team (NRT) is an organization of 15 Federal departments and agencies responsible for coordinating emergency preparedness and response to oil and hazardous substance pollution incidents.
<a href="#">RAPIDTOX1</a>	<a href="#">RAPIDTOX: Test1 Emergency Responder</a>	2019-06-08	3988	Test Interface with data for emergency responders
<a href="#">WEBWISER</a>	<a href="#">LIST: WEBWISER</a>	2019-04-13	449	WISER is a system designed to assist emergency responders in hazardous material incidents.

5 records



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# Emergency Response List

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

### US National Response Team Chemical Set

Search NRTCHEMICALS Chemicals

☐ Identifier substring search

**List Details**

**Description:** The U.S. National Response Team (NRT) is an organization of 15 Federal departments and agencies responsible for coordinating emergency preparedness and response to oil and hazardous substance pollution incidents. The Environment Protection Agency (EPA) and the U.S. Coast Guard (USCG) serve as Chair and Vice Chair respectively. The National Oil and Hazardous Substances Pollution Contingency Plan (NCP) and the Code of Federal Regulations (40 CFR part 300) outline the role of the NRT and Regional Response Teams (RRTs). The response teams are also cited in various federal statutes, including Superfund Amendments and Reauthorization Act (SARA) – Title III and the Hazardous Materials Transportation Act [HMTA]. The chemicals list here is sourced from the [Chemical Hazards Page](#)

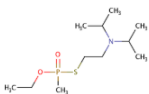
**Number of Chemicals:** 18

18 chemicals

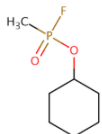
Select all Download Send to Batch Search Default CASRN DTXSID Mono.Mass Hide chemicals that are Filter by Name or CASRN

1 related chemical structure with this substance

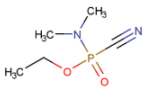
Cyanide salts  
CASRN:NOCAS\_872420  
DTXSID:DTXSID40872420  
Mono.Mass:0



VX  
CASRN:50782-69-9  
DTXSID:DTXSID80866161  
Mono.Mass:267.142187



Cyclosarin  
CASRN:329-99-7  
DTXSID:DTXSID00861875  
Mono.Mass:180.071545



Tabun  
CASRN:77-81-6  
DTXSID:DTXSID80861631  
Mono.Mass:162.055815

# WebWISER List

## LIST: WEBWISER

Search WEBWISER Chemicals

Identifier substring search

### List Details

**Description:** WISER is a system designed to assist emergency responders in hazardous material incidents. WISER provides a wide range of information on hazardous substances, including substance identification support, physical characteristics, human health information, and containment and suppression advice.

**Number of Chemicals:** 449

Select all

Download

Send to Batch Search

Default



4 chemicals

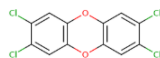
CASRN

DTXSID

Mono.Mass

Hide chemicals that are:

tetrachloro

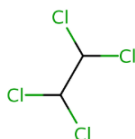


2,3,7,8-Tetrachlorodibenzo-p-dioxin

CASRN:1746-01-6

DTXSID:DTXSID2021315

Mono.Mass:319.89654

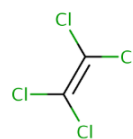


1,1,2,2-Tetrachloroethane

CASRN:79-34-5

DTXSID:DTXSID7021318

Mono.Mass:165.891061

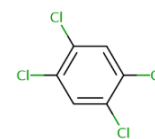


Tetrachloroethylene

CASRN:127-18-4

DTXSID:DTXSID2021319

Mono.Mass:163.875411



1,2,4,5-Tetrachlorobenzene

CASRN:95-94-3

DTXSID:DTXSID7024320

Mono.Mass:213.891061

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

# ***Batch Searching***



- Singleton searches are useful but people generally want data on LOTS of chemicals!
- Typical questions
  - What is the list of chemicals for the formula  $C_xH_yO_z$
  - What is the list of chemicals for a mass +/- error
  - Can I get chemical lists in Excel files? In SDF files?
  - Can I include properties in the download file?

# Batch Search Names

Buprenorphine  
Codeine  
Dextromethorphan  
Dihydrocodeine  
Dihydromorphine  
Ethylmorphine  
Fentanyl  
Heroin  
Hydrocodone  
Hydromorphone  
Ketamine  
Meperidine  
Methadone  
Morphine  
Morphinone  
Naloxone  
Naltriben  
Oxycodone  
Oxymorphone  
Propoxyphene  
Sufentanil  
Tramadol

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

Step Five: Choose Data Fields to Download

Please enter one identifier per line

Select Input Type(s)

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

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

Buprenorphine  
Codeine  
Dextromethorphan  
Dihydrocodeine  
Dihydromorphine  
Ethylmorphine  
Fentanyl  
Heroin  
Hydrocodone  
Hydromorphone

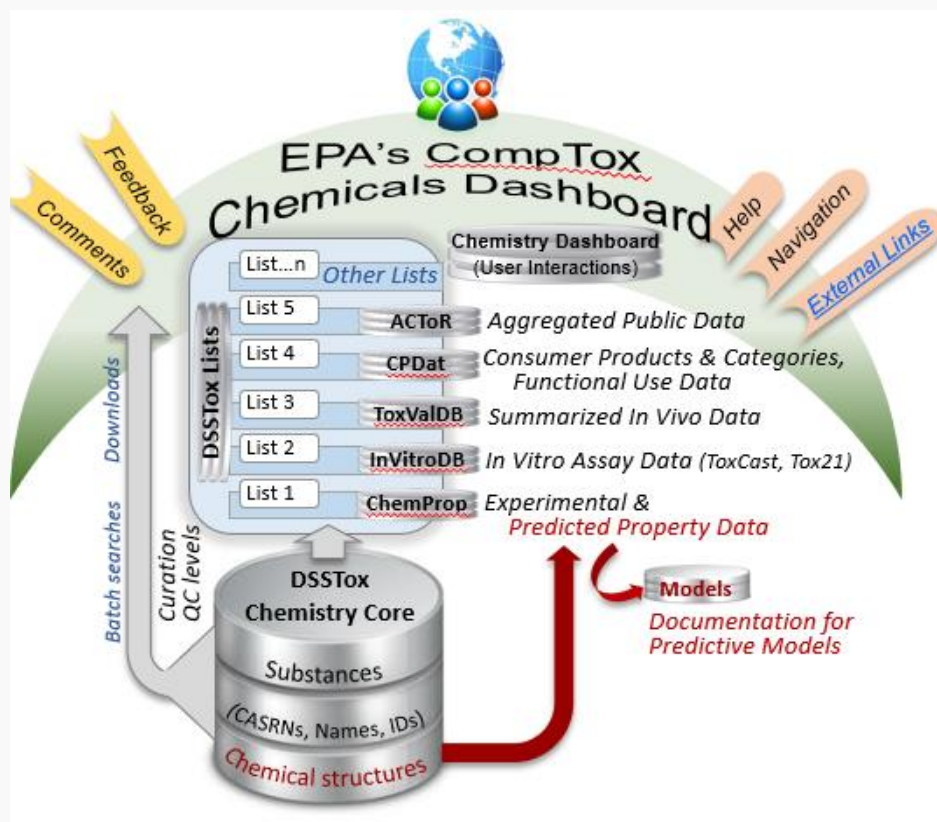
Display All Chemicals      Download Chemical Data

Excel  
Download

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

# Conclusion

- An integrated hub for environmental chemistry data to serve computational toxicology
- Serving multiple use cases and needs – let's talk!

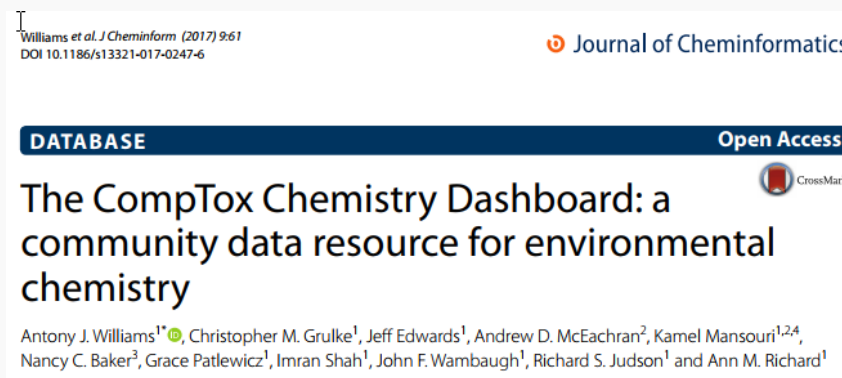


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<https://doi.org/10.1186/s13321-017-0247-6>