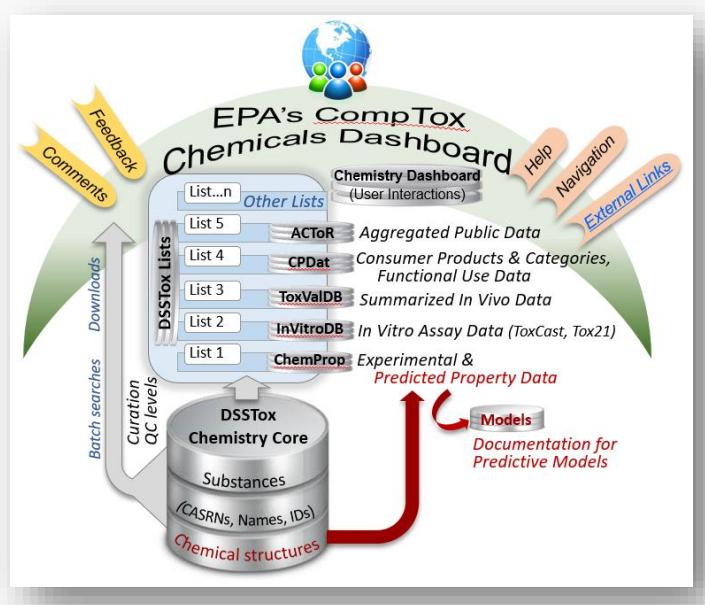


EPA CompTox Chemicals Dashboard as a Data Integration Hub for Environmental Chemistry Data



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

*November 2019
Decontamination Conference, Norfolk, VA*

CompTox Chemicals Dashboard

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



- **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 single application integrating...

The image is a collage of screenshots from the EPA's Toxics Release Inventory (TRI) and Chemicals databases, illustrating various search, analysis, and data visualization features. The screenshots are arranged in a grid-like structure, each showing a different aspect of the platform's functionality.

- Top Left:** A search bar for "785 Thousand Chemicals" with a "SEARCH" button. Below it is a "Batch Search" interface titled "BATCH SEARCH" with a progress bar and a list of chemical identifiers.
- Top Center:** A "Hazard" page for Bisphenol A (80-05-7) showing toxicity data across various exposure routes and environmental media.
- Top Right:** A "TOX DATA" section for Bisphenol A, featuring a "BIOACTIVITY" chart showing chemical activity summary data.
- Middle Left:** A "SIMILARITY" page for Bisphenol A, showing a grid of chemical structures and their similarity scores.
- Middle Center:** A "Step Three: Run GenRA Prediction" page showing a network of chemical structures and a heatmap of predicted bioactivities.
- Middle Right:** A "TOXCAST" page for Bisphenol A, displaying a scatter plot of toxicity data.
- Bottom Left:** A "RELATED SUBSTANCES" page for Bisphenol A, showing a network of related chemical structures.
- Bottom Center:** A "SYNTHONS" page for Bisphenol A, showing a network of chemical structures and their synthesis routes.
- Bottom Right:** A "TOXCAST" page for Bisphenol A, showing a scatter plot of toxicity data.

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>



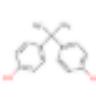
875k Chemical Substances

The screenshot shows the CompTox Chemicals Dashboard homepage. At the top, the EPA logo is on the left, followed by the text "United States Environmental Protection Agency". To the right are navigation links: Home, Advanced Search, Batch Search, Lists, Predictions, and Downloads. On the far right is a "Share" button. The main title "875 Thousand Chemicals" is centered above a search bar. The search bar has three tabs: "Chemicals" (which is selected and highlighted in blue), "Product/Use Categories", and "Assay/Gene". Below the search bar is a search input field with placeholder text "Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey" and a checkbox for "Identifier substring search". To the right of the search bar, there is a message: "See what people are saying, read the dashboard [comments](#)! Cite the Dashboard Publication [click here](#)". Below this is a section titled "Latest News" with a link to "Read more news". A news item is displayed: "Journal of Cheminformatics article regarding 'MS-Ready structures'" with a timestamp "March 9th, 2019 at 1:09:45 PM". The text of the news item reads: "A recent article describes 'MS-Ready structures', what they are, how they are generated and details regarding the benefits of these structures in navigating structure relationships across the dashboard. The article is published in the Journal of Cheminformatics [here](#)". Navigation arrows and a horizontal ellipsis are at the bottom of the news section.

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

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:** $\text{C}_{15}\text{H}_{16}\text{O}_2$  

 **Average Mass:** 228.291 g/mol 

 **Monoisotopic Mass:** 228.11503 g/mol

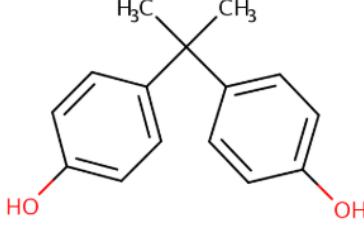
Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Quality Control Notes



The chemical structure of Bisphenol A is shown as a central carbon atom bonded to two methyl groups (CH_3) and two hydroxyphenyl groups. Each hydroxyphenyl group consists of a benzene ring attached to a hydroxyl group (OH) at the para position relative to the central carbon atom.

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 36) and was positive in 9 AR assays (tested in 19).

ADME

- ✓ HTTK Css 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

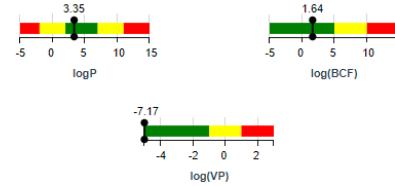
Other Notes

- ✗ 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 |

PHYSCHEM PARAMETERS



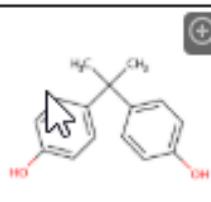
Quantitative Risk Assessment Values

- ✓ IRIS values available [🔗](#)
- ✗ No PPRTV values
- ✓ EPA RSL values available [🔗](#)
- ✓ Minimum RfD: 0.050 mg/kg-day (chronic, IRIS, oral, 8) [🔗](#)
- ✗ 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, 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 |
|---------------------|----------------------|-------------------|
| LogP: Octanol-Water | 3.32 (1) | 3.29 |
| Melting Point | 155 (7) | 139 |
| Boiling Point | 200 (1) | 363 |
| Water Solubility | 5.26e-4 (1) | 9.62e-4 |
| Vapor Pressure | - | 8.37e-7 |
| Flash Point | - | 190 |

Transparency for prediction models



Predicted

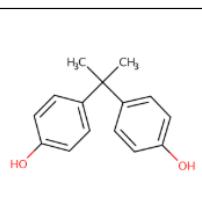
 Download Predicted Data ▾

| Source | Result | Calculation Details | QMRF |
|--------------------|--------|--|---------------|
| EPISUITE | 3.64 | Not Available | Not Available |
| NICEATM | 2.40 | Not Available | Available |
| ACD/Labs Consensus | 3.63 | Not Available | Not Available |
| ACD/Labs | 3.43 | Not Available | Not Available |
| OPERA | 3.35 | OPERA Model Report [Inside AD] | Available |

OPERA Models: LogP: Octanol-Water

Bisphenol A

80-05-7 | DTXSID7020182

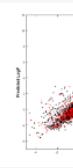
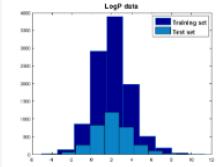


Model Results

Predicted value: 3.35
Global applicability domain: Inside
Local applicability domain index: 0.877
Confidence level: 0.813

 Print PDF

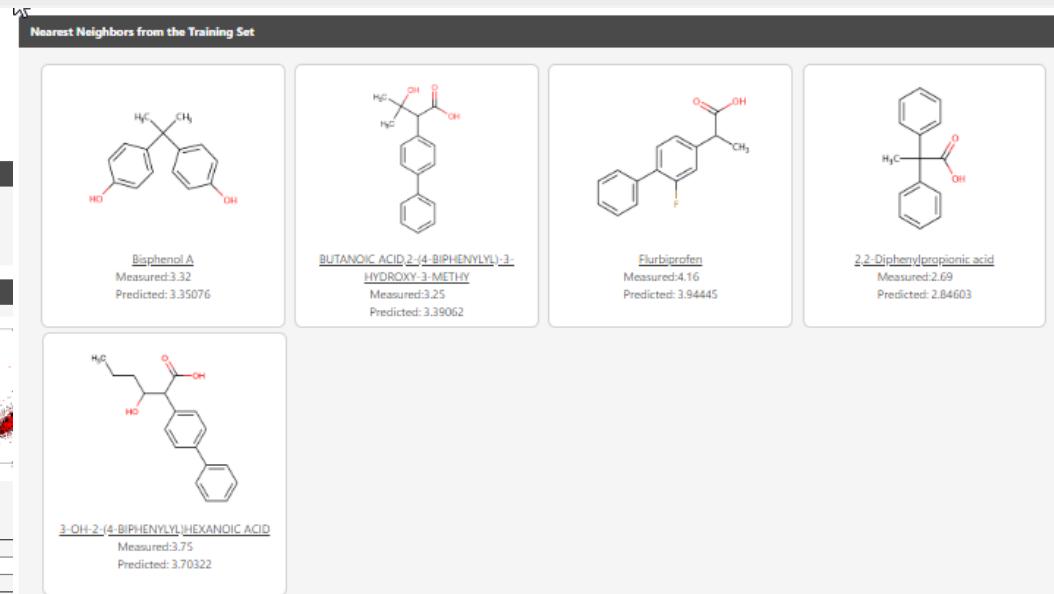
Model Performance



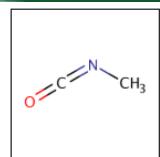
 QMRF

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | |
|-----------------|-------|----------------|-------|
| Q2 | RMSE | R2 | RMSE |
| 0.850 | 0.690 | 0.860 | 0.670 |



Access to Chemical Hazard Data



Methyl isocyanate

624-83-9 | DTXSID1023786

Searched by DSSTox Substance Id.

Hazard

DataType

Toxicity Value



 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 | Pennsylvania DEP ToxValues |
|  | AEGL 2 - 8 hr (final) | acute | 0.008 | ppm | inhalation | EPA OW | EPA AEGL |
|  | MEG | short-term | 0.016 | mg/m3 | inhalation | TG 230 Military Exposure Guidelines Table | DOD |
|  | MEG | chronic | 0.016 | mg/m3 | inhalation | TG 230 Military Exposure Guidelines Table | DOD |
|  | AEGL 2 - 4 hr (final) | acute | 0.017 | ppm | inhalation | EPA OW | EPA AEGL |
|  | MEG | short-term | 0.02 | mg/m3 | inhalation | TG 230 Military Exposure Guidelines Table | DOD |
|  | MEG | short-term | 0.02 | mg/m3 | inhalation | TG 230 Military Exposure Guidelines Table | DOD |
|  | AEGL 3 - 8 hr (final) | acute | 0.025 | ppm | inhalation | EPA OW | EPA AEGL |
|  | AEGL 3 - 4 hr (final) | acute | 0.05 | ppm | inhalation | EPA OW | EPA AEGL |
|  | MEG | short-term | 0.058 | mg/m3 | inhalation | TG 230 Military Exposure Guidelines Table | DOD |

Hazard Data from “ToxVal_DB”



- 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 Search all data

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

Product and Use Categories (PUCs)

Download Columns 10 Search query

| 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

Sources of Exposure to Chemicals

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

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 |
|---|-------------------|-------------------|
| 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

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

SYNOMYNS

► LITERATURE

LINKS

COMMENTS

25

Synonym

Bisphenol A

4,4'-(Propane-2,2-diyl)diphenol

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

80-05-7 Active CAS-RN

BPA

4,4'-Propane-2,2-diylidiphenol

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

4-06-00-06717 Beilstein Registry Number

(4,4'-Dihydroxydiphenyl)dimethylmethane

2,2-Bis(4-hydroxyphenyl)propane

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

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

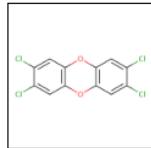
2,2-Bis(4-hydroxyphenyl)propane

2,2-Bis(p-hydroxyphenyl)propane

2,2-Di(4-Hydroxyphenyl) Propane

Search query

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](#)
-  [CCCRIS](#)
-  [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 IR Spectrum](#)
-  [NIST MS Spectrum](#)
-  [MassBank](#)
-  [NEMI: National Environmental Methods Index](#)
-  [NIST Antoine Constants](#)
-  [IR Spectra on PubChem](#)
-  [NIST Kovats Index values](#)
-  [Protein DataBank](#)

Prediction

-  [2D NMR HSQC/HMBC Prediction](#)
-  [Carbon-13 NMR Prediction](#)
-  [Proton NMR Prediction](#)
-  [LSERD](#)

External Links

 **WEBWISER**

 [PubChem Safety Sheet](#)

 [NIOSH Chemical Safety Cards](#)

 U.S. National Library of Medicine
Specialized Information Services



**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.

External Links

 **WEBWISER**

 **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 | <u>Danger</u> Aggregated GHS information provided by 23 companies from 1 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies. H300 (100%): Fatal if swallowed [<u>Danger</u> Acute toxicity, oral] H319 (100%): Causes serious eye irritation [<u>Warning</u> Serious eye damage/eye irritation] H400 (100%): Very toxic to aquatic life [<u>Warning</u> Hazardous to the aquatic environment, acute hazard] H410 (100%): Very toxic to aquatic life with long lasting effects [<u>Warning</u> Hazardous to the aquatic environment, long-term hazard] 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. |
| GHS Hazard Statements | |

External Links



PubChem Safety Sheet

NIOSH Chemical Safety Cards

[« back to the search result list](#)

English - EN ▾

ICSC: 1467

November 2003

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

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

2,3,7,8-TCDD

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

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. |

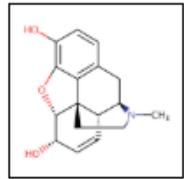
AVOID ALL CONTACT! IN ALL CASES CONSULT A DOCTOR!

| | 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 |
| STORAGE | Transportation UN Classification UN Hazard Class: 6.1; UN Pack Group: I |
| Separated from food and feedstuffs. | |
| PACKAGING | |

Built in “Modules”

Literature Searching



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 

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

Retrieve Articles

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)
```

Literature Searching

37 of 37 articles loaded...

To find articles quickly, enter terms to sift abstracts. 

wastewater

Spectrometry

EPA

Clear Terms

Download / Send to... 

 **Download Sifter for Excel** 

| | wastewater | Spectrometry  | EPA | Total | PMID | Year | Title | Authors | Journal | Rev |
|--|------------|--|-----|-------|----------|------|---|--|---|-----|
| | 4 | 2 | 0 | 6 | 29274731 | 2017 | Simultaneous analysis of opioid analgesics and thei... | Krizman-Matasic; Kostanjevecki; Ahel; Terzic | Journal of chromatography. A | |
| | 0 | 1 | 0 | 1 | 25768972 | 2015 | Evaluating external contamination of polybrominate... | Poon; Alekса; Carnevale; Kapur; Goodyer; Koren | Therapeutic drug monitoring | |
| | 0 | 1 | 0 | 1 | 22544551 | 2012 | Spatial distribution of illicit drugs in surface waters o... | Vazquez-Roig; Andreu; Blasco; Morillas; Picó | Environmental science and pollution research inter... | |
| | 1 | 1 | 0 | 2 | 20801487 | 2010 | Analysis of illicit and illicit drugs in waste, surface an... | Berset; Brenneisen; Mathieu | Chemosphere | |
| | 1 | 1 | 0 | 2 | 17935751 | 2007 | Illicit drugs, a novel group of environmental contami... | Zuccato; Castiglioni; Bagnati; Chiabrando; Grassi; ... | Water research | |
| | 2 | 1 | 1 | 4 | 17607391 | 2007 | Using environmental analytical data to estimate lev... | Bones; Thomas; Paull | Journal of environmental monitoring : JEM | |
| | 3 | 1 | 2 | 6 | 17180984 | 2006 | Simultaneous determination of psychoactive drugs ... | Hummel; Löffler; Fink; Ternes | Environmental science & technology | |
| | 6 | 0 | 0 | 6 | 30583189 | 2018 | Assessment of drugs of abuse in a wastewater trea... | Kumar; Tscharke; O'Brien; Mueller; Wilkins; Padhye | The Science of the total environment | |
| | 0 | 0 | 3 | 3 | 30488421 | 2018 | Effect of enriched environment during adolescence ... | Mohammadian; Najafi; Miladi-Gorji | Developmental psychobiology | |
| | 3 | 0 | 0 | 3 | 29574368 | 2018 | Estimation of the consumption of illicit drugs during ... | Foppe; Hammond-Weinberger; Subedi | The Science of the total environment | |
| | 1 | 0 | 0 | 1 | 28787791 | 2017 | Evaluation of in-sewer transformation of selected illi... | Gao; Banks; Li; Jiang; Lai; Mueller; Thai | The Science of the total environment | |
| | 9 | 0 | 0 | 9 | 28472697 | 2017 | Occurrence and fate of illicit drugs and pharmaceuti... | Causanilles; Ruepert; Ibáñez; Emke; Hernández; d... | The Science of the total environment | |
| | 0 | 0 | 0 | 0 | 28010888 | 2016 | Dose-dependent effects of morphine on lipopolysac... | Mottaz; Schönenberger; Fischer; Eggen; Schirmer; ... | Environmental pollution (Barking, Essex : 1987) | |
| | 0 | 0 | 0 | 0 | 27746311 | 2016 | Effects of voluntary exercise on the viability, prolifer... | Haydari; Safari; Zarbakhsh; Bandegi; Miladi-Gorji | Neuroscience letters | |
| | 0 | 0 | 0 | 0 | 27261879 | 2016 | Genotoxic effects induced by the exposure to an en... | Parolini; Magni; Castiglioni; Binelli | Ecotoxicology and environmental safety | |
| | 3 | 0 | 0 | 3 | 27179320 | 2016 | Temporal trends in drug use in Adelaide, South Aus... | Tscharke; Chen; Gerber; White | The Science of the total environment | |

Chemical Lists

EPAHFR: Hydraulic Fracturing



United States Environmental Protection Agency

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Select List

Download Columns emergency Copy Filtered Lists URL

| List Acronym | List Name | Last Updated | Number of Chemicals | List Description |
|--------------|---|--------------|---------------------|--|
| 40CFR355 | 40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities | 2018-01-05 | 354 | Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378) |
| HAZSUBST | WIKILIST: Extremely hazardous substances | 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) |
| NRTCHEMICALS | US National Response Team Chemical Set | 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. |
| RAPIDTOX1 | RAPIDTOX: Test1 Emergency Responder | 2019-06-08 | 3988 | Test Interface with data for emergency responders |
| WEBWISER | LIST: WEBWISER | 2019-04-13 | 449 | WISER is a system designed to assist emergency responders in hazardous material incidents. |

5 records

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

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Emergency Response List

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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 Environmental 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 ▾    Hide chemicals that are: ▾ Filter by Name or CASRN 

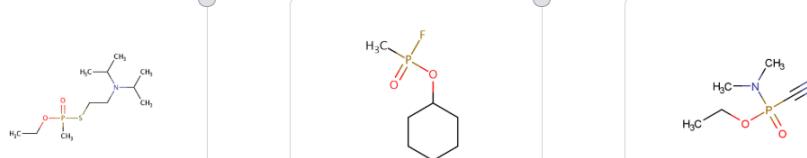
1 related chemical structure with this substance

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

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

LIST: WEBWISER

Search WEBWISER Chemicals Identifier substring search

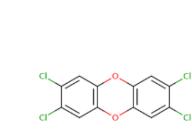
List Details

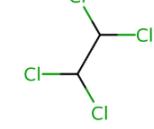
Description: WISER is a system designed to assist emergency responders in hazardous material incidents. WISER provides a wide range of information on hazardous substances, including substance identification support, physical characteristics, human health information, and containment and suppression advice.

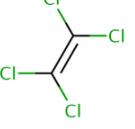
Number of Chemicals: 449

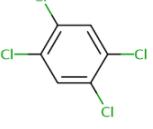
4 chemicals

Select all  Download ▾ Send to Batch Search Default  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

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 x

Select Input Type(s)

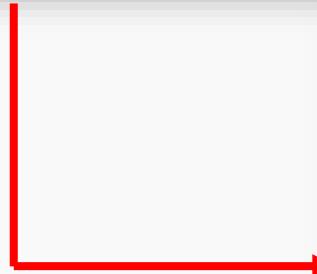
Identifiers
 Chemical Name i
 CASRN i
 InChIKey i
 DSSTox Substance ID i
 DSSTox Compound ID i
 InChIKey Skeleton i
 MS-Ready Formula(e) i
 Exact Formula(e) i
 Monoisotopic Mass i

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

Buprenorphine
Codeine
Dextromethorphan
Dihydrocodeine
Dihydromorphine
Ethylmorphine
Fentanyl
Heroin
Hydrocodone
Hydromorphone

Display All Chemicals ... Download Chemical Data

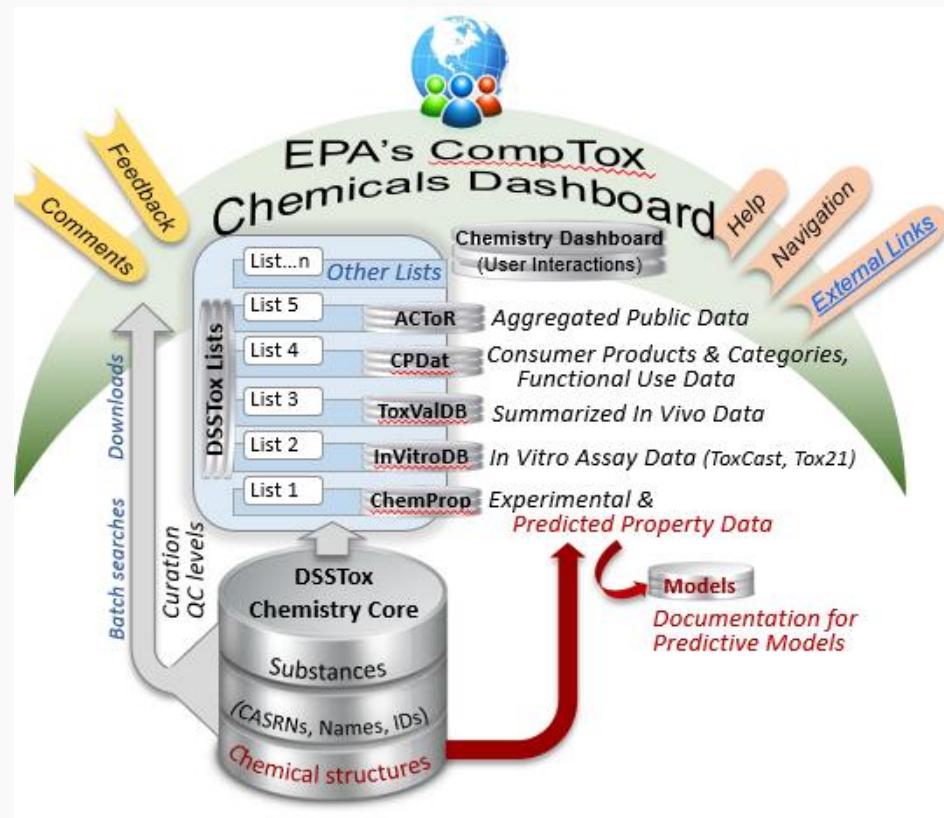
Excel
Download



| INPUT | FOUND_BY | DTXSID |
|------------------|---------------|---------------|
| Buprenorphine | Approved Name | DTXSID2022705 |
| Codeine | Approved Name | DTXSID2020341 |
| Dextromethorphan | Approved Name | DTXSID3022908 |
| Dihydrocodeine | Approved Name | DTXSID5022936 |
| Dihydromorphine | Approved Name | DTXSID7048908 |
| Ethylmorphine | Approved Name | DTXSID1046760 |
| Fentanyl | Approved Name | DTXSID9023049 |
| Heroin | Synonym | DTXSID6046761 |
| Hydrocodone | Approved Name | DTXSID8023131 |
| Hydromorphone | Approved Name | DTXSID8023133 |
| Ketamine | Approved Name | DTXSID8023187 |
| Meperidine | Approved Name | DTXSID9023253 |
| Methadone | Approved Name | DTXSID7023273 |
| Morphine | Approved Name | DTXSID9023336 |
| Tramadol | Approved Name | DTXSID5040807 |

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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DOI 10.1186/s13321-017-0247-6

 **Journal of Cheminformatics**

DATABASE **Open Access** 

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

Antony J. Williams¹ , Christopher M. Grolke¹, Jeff Edwards¹, Andrew D. McEachran², Kamel Mansouri^{1,2,4}, Nancy C. Baker³, Grace Patlewicz¹, Imran Shah¹, John F. Wambaugh¹, Richard S. Judson¹ and Ann M. Richard¹

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