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

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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...

- Batch Search
- Tox Data
- Bioactivity
- Similarity

Graphical user interface showing search and data analysis features.
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
875k Chemical Substances
BASIC Search

Search for 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)
Bisphenol A (BPA) is an organic synthetic compound with the chemical formula \( \text{C}_{15}\text{H}_{14}\text{O}_{2} \), belonging to the group of dihydroxydiphenyl ethers and bisphenols with two hydroxyl 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.

**Intrinsic Properties**

- **Molecular Formula**: \( \text{C}_{15}\text{H}_{14}\text{O}_{2} \)
- **Mol Wt**: 228.221 g/mol

**Structural Identifiers**

**Linked Substances**

**Presence In Lists**

**Record Information**

**Quality Control Notes**
An “Executive Summary”
Quick Look Tox Info

**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 RFC calculated
- IVIVE POD not calculated

**Cancer Information**
- No cancer slope factor
- No inhalation risk value
- Carcinogenicity data available: University of Maryland carcinogenicity warning

**Reproductive Toxicology**
- 240 Reproductive toxicity PODs available

**Chronic Toxicology**
- 249 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 neurotoxicity data available.

**Endocrine System**
- Endocrine Disruption Potential: Significant Estrogen and Androgen-Receptor activity seen.

**ADME**
- HTTK data are available

**Fate and Transport**
- No bioaccumulation concern
- 60% of values available

**Exposure**
- Exposure estimates are available based on NMEP and SEEM

**AOP Information**
- AOP Level: 13, 33, 36, 58, 84, 99, 107, 124, 180, 183, 187, 187, 200

**Other Notes**
- No other quality values available
- No air quality values available
- 14 Occupational exposure values available

**Regional Screening**

<table>
<thead>
<tr>
<th>Class</th>
<th>THQ</th>
<th>Value</th>
</tr>
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<tbody>
<tr>
<td>risk-based SSL (mg/kg)</td>
<td>THQ &gt; 1</td>
<td>5.0</td>
</tr>
<tr>
<td>GI/BS (unspecified)</td>
<td>THQ &gt; 1</td>
<td>1.0</td>
</tr>
<tr>
<td>GI/BS (unspecified)</td>
<td>THQ &gt; 1</td>
<td>1.0</td>
</tr>
<tr>
<td>GI/BS (specified)</td>
<td>THQ &gt; 1</td>
<td>0.1</td>
</tr>
<tr>
<td>screening test (toxicokinetic)</td>
<td>THQ &gt; 1</td>
<td>10.0</td>
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<td>10.0</td>
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<td>10.0</td>
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<td>THQ &gt; 1</td>
<td>10.0</td>
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<td>screening level (toxicokinetic)</td>
<td>THQ &gt; 1</td>
<td>10.0</td>
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<td>THQ &gt; 1</td>
<td>10.0</td>
</tr>
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**Lowest Observed Bioactivity Equivalent Level: CYP1A1, CYP1A2, Topo, Esr1, NR113, PPAR, NR112, Cy2c11, MMP3, Esr1**
### Experimental and Predicted Data

#### Bisphenol A

**Experimental and Predicted Data**

<table>
<thead>
<tr>
<th>Property</th>
<th>Experimental average</th>
<th>Predicted average</th>
</tr>
</thead>
<tbody>
<tr>
<td>LogP: Octanol-Water</td>
<td>3.32 (1)</td>
<td>3.29</td>
</tr>
<tr>
<td>Melting Point</td>
<td>155 (7)</td>
<td>139</td>
</tr>
<tr>
<td>Boiling Point</td>
<td>200 (1)</td>
<td>363</td>
</tr>
<tr>
<td>Water Solubility</td>
<td>5.26e-4 (1)</td>
<td>9.62e-4</td>
</tr>
<tr>
<td>Vapor Pressure</td>
<td>-</td>
<td>8.37e-7</td>
</tr>
<tr>
<td>Flash Point</td>
<td>-</td>
<td>190</td>
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</table>
Transparency for prediction models

## Predicted Data

<table>
<thead>
<tr>
<th>Source</th>
<th>Result</th>
<th>Calculation Details</th>
<th>QMRF</th>
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</thead>
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<tr>
<td>EPISUITE</td>
<td>3.64</td>
<td>Not Available</td>
<td>Not Available</td>
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<tr>
<td>NICEATM</td>
<td>2.40</td>
<td>Not Available</td>
<td>Available</td>
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<tr>
<td>ACD/Labs Consensus</td>
<td>3.63</td>
<td>Not Available</td>
<td>Not Available</td>
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<tr>
<td>ACD/Labs</td>
<td>3.43</td>
<td>Not Available</td>
<td>Not Available</td>
</tr>
<tr>
<td>OPERA</td>
<td>3.35</td>
<td>[OPERA Model Report (inside AD)]</td>
<td>Available</td>
</tr>
</tbody>
</table>

### OPERA Models: LogP: Octanol-Water

**Bisphenol A**

80-05-7 | DTXSID7020182

**Model Results**

- Predicted value: 3.35
- Local hydrophobic density: 1.36
- Local hydrophobic density: 3.47
- Standard error: 0.13

**Model Performance**

- LogP vs. Predicted

**Nearest Neighbors from the Training Set**

1. Bisphenol A
   - Measured: 3.26
   - Predicted: 3.30

2. 2,4-Dinitrophenylhydrazine
   - Measured: 2.82
   - Predicted: 2.82

3. 3-OH-2-4-DIPHENYLEDICARBOXYLBENZENEFumarate
   - Measured: 3.07
   - Predicted: 3.07
### Access to Chemical Hazard Data

#### Methyl isocyanate

**624-83-9 | DTXSID1023786**

Searched by DSSTox Substance Id.

**Hazard**

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

Bisphenol A
80-05-7 | DTXSID7020182

Chemical Activity Summary

AC50 (μM): 48.35
Scaled log: 6.19
Assay Endpoint Name: TCX1_CAR_Agonist
Gene Symbol: NR1B
Organism: Human
Tissue: Liver
Assay Format Type: cell-based
Biological Process Target: regulation of transcription factor activity
Detection Technology: luminescence-coupled ATP quantitation
Analysis Direction: positive
Intended Target Family: nuclear receptor
Description: Data from the assay component TCX1_CAR_Agonist was analyzed into 1 assay endpoint. This assay endpoint, TCX1_CAR_Agonist, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of relative reporter, gain-of-signal activity, can be used to understand changes in the reporter gene as they relate to the gene NR1B. Furthermore, this assay endpoint can be referred to as a primary method because the performed assay has only produced 1 assay endpoint. To generalize the intended target to other relevant targets, this assay endpoint is annotated to the nuclear receptor intended target family.
Sources of Exposure to Chemicals

Bisphenol A
80-05-7 | DTXSID7020182
Searched by DSSTox Substance Id.

Product and Use Categories (PUCs)

<table>
<thead>
<tr>
<th>Product or Use Categorization</th>
<th>Categorization type</th>
<th>Number of Unique Products</th>
</tr>
</thead>
<tbody>
<tr>
<td>manufacturing, metals</td>
<td>CPCat Cassette</td>
<td>17</td>
</tr>
<tr>
<td>adhesive</td>
<td>CPCat Cassette</td>
<td>17</td>
</tr>
<tr>
<td></td>
<td>CPCat Cassette</td>
<td>15</td>
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<tr>
<td></td>
<td>CPCat Cassette</td>
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<tr>
<td></td>
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<tr>
<td></td>
<td>CPCat Cassette</td>
<td>8</td>
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<tr>
<td></td>
<td>CPCat Cassette</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>CPCat Cassette</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>CPCat Cassette</td>
<td>7</td>
</tr>
<tr>
<td></td>
<td>CPCat Cassette</td>
<td>6</td>
</tr>
</tbody>
</table>

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.

Toxics Release Inventory

2015 TRI Factsheet: Chemical - 4,4'-ISOPROPYLDENEDIPHENOL, 000080057
Data Source: 2015 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'-ISOPROPYLDENEDIPHENOL

Quick Facts for 2015

<table>
<thead>
<tr>
<th></th>
<th>Chemical</th>
<th>United States</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of TRI Facilities:</td>
<td>120</td>
<td>22,130</td>
</tr>
<tr>
<td>Total Production-Related Waste Managed:</td>
<td>15.8 million lbs</td>
<td>27.1 billion lbs</td>
</tr>
<tr>
<td>Total On-site and Off-site Disposal or Other Releases:</td>
<td>2.5 million lbs</td>
<td>3.4 billion lbs</td>
</tr>
<tr>
<td>Total On-site:</td>
<td>39.4 thousand lbs</td>
<td>2.9 billion lbs</td>
</tr>
<tr>
<td>Air:</td>
<td>28.7 thousand lbs</td>
<td>686.4 million lbs</td>
</tr>
<tr>
<td>Water:</td>
<td>4.4 thousand lbs</td>
<td>198.2 million lbs</td>
</tr>
<tr>
<td>Land:</td>
<td>6.2 thousand lbs</td>
<td>2.0 billion lbs</td>
</tr>
</tbody>
</table>
Identifiers to Support Searches

Bisphenol A
80-05-7 | DTXSID7020182
Searched by DSSTox Substance Id.

**Synonym**

- Bisphenol A
- 4,4'-Propane-2,2-diylidiphenol
- Phenol, 4,4'-[1-methylene]bis-

**Details**

- Quality: Valid
- Exact Mass: 256.089
- Molecular Formula: C16H14O2
- Molecular Weight: 256.243
- CAS Number: 80-05-7
- Exact Mass Measurement: So
- Exact Mass Measurement: Good
- Molecular Formula: Exact Mass Measurement: So
- Molecular Weight: Exact Mass Measurement: Good
- Exact Mass Measurement: So
- Molecular Formula: Exact Mass Measurement: Good
- Molecular Weight: Exact Mass Measurement: Good
- Exact Mass Measurement: So
- Molecular Formula: Exact Mass Measurement: Good
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- Molecular Formula: Exact Mass Measurement: Good
- Molecular Weight: Exact Mass Measurement: Good
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- Molecular Formula: Exact Mass Measurement: Good
- Molecular Weight: Exact Mass Measurement: Good
- Exact Mass Measurement: So
- Molecular Formula: Exact Mass Measurement: Good
- Molecular Weight: Exact Mass Measurement: Good
- Exact Mass Measurement: So
- Molecular Formula: Exact Mass Me
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
- CPCM
- 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
- SCRIS
- 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
- m2Cloud
- 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/HMB Prediction
- Carbon-13 NMR Prediction
- Proton NMR Prediction
- LSERD
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.
2,3,7,8-Tetrachlorodibenzo-P-dioxin

GHS Classification

Showing 3 of 3

Pictogram(s)

- Acute Toxic
- Irritant
- Environmental Hazard

Signal

 Danger

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 [Danger Acute toxicity, oral]

H319 (100%): Causes serious eye irritation [Warning Serious eye damage/eye irritation]

H400 (100%): Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard]

H410 (100%): Very toxic to aquatic life with long lasting effects [Warning 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.
<table>
<thead>
<tr>
<th><strong>External Links</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>WEBWISER</td>
</tr>
<tr>
<td>PubChem Safety Sheet</td>
</tr>
<tr>
<td>NIOSH Chemical Safety Cards</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Chemical Safety Sheet</strong></th>
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<td><strong>CAS #</strong>: 1746-01-6</td>
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<td><strong>UN #</strong>: 2811</td>
</tr>
<tr>
<td><strong>EC Number</strong>: 217-122-7</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>2,3,7,8-TETRACHLORODIBENZO-(p)-DIOXIN</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Dibenzo ([b,e]) (1,4)dioxin, 2,3,7,8-tetrachloro-</td>
</tr>
<tr>
<td>2,3,7,8-TCDD</td>
</tr>
<tr>
<td>2,3,7,8-Tetrachloro-1,4-dioxin</td>
</tr>
<tr>
<td><strong>ICSC</strong>: 1467</td>
</tr>
<tr>
<td><strong>November 2003</strong></td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>ACUTE HAZARDS</strong></th>
<th><strong>PREVENTION</strong></th>
<th><strong>FIRE FIGHTING</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>FIRE &amp; EXPLOSION</td>
<td>Gives off irritating or toxic fumes (or gases) in a fire.</td>
<td>In case of fire in the surroundings, use appropriate extinguishing media.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>AVOID ALL CONTACT! IN ALL CASES CONSULT A DOCTOR!</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>SYMPTOMS</strong></td>
</tr>
<tr>
<td><strong>INHALATION</strong></td>
</tr>
<tr>
<td>Symptoms may be delayed.</td>
</tr>
<tr>
<td><strong>SKIN</strong></td>
</tr>
<tr>
<td><strong>EYES</strong></td>
</tr>
<tr>
<td>Redness. Pain.</td>
</tr>
<tr>
<td><strong>INGESTION</strong></td>
</tr>
<tr>
<td>See Inhalation.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>FIRST AID</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>INHALATION</strong></td>
</tr>
<tr>
<td>Fresh air, rest. Refer for medical attention.</td>
</tr>
<tr>
<td><strong>SKIN</strong></td>
</tr>
<tr>
<td>Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer for medical attention.</td>
</tr>
<tr>
<td><strong>EYES</strong></td>
</tr>
<tr>
<td>First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.</td>
</tr>
<tr>
<td><strong>INGESTION</strong></td>
</tr>
<tr>
<td>Give a slurry of activated charcoal in water to drink. Induce vomiting (ONLY IN CONSCIOUS PERSONS!). Refer for medical attention.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>SPILLAGE DISPOSAL</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Evacuate danger area! Consult an expert! Personal protection: chemical protection suit including self-contained breathing apparatus.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>CLASSIFICATION &amp; LABELLING</strong></th>
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<tbody>
<tr>
<td>According to UN GHS Criteria</td>
</tr>
<tr>
<td><strong>STORAGE</strong></td>
</tr>
<tr>
<td>Transportation</td>
</tr>
<tr>
<td>UN Classification</td>
</tr>
<tr>
<td>UN Hazard Class: 6.1; UN Pack Group: 1</td>
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</tbody>
</table>
Built in “Modules”
Literature Searching

Morphine
57-27-2 | DTXSID9023336

Abstract Sifter

1) Select PubMed starting point query then 2) click on Retrieve.  
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)
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<th>EPA</th>
<th>Total</th>
<th>PMID</th>
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<th>Title</th>
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<td>Simultaneous analysis of opioid analgesics and their metabolites...</td>
<td>Krizman-Matasic, Kostanjsekovic, Alme, Terzić</td>
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<td>Spatial distribution of illicit drugs in surface waters...</td>
<td>Vazquez-Roig, Andreu, Elsaco, Morillas, Piqué</td>
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<td>Analysis of illicit and illicit drugs in waste, surface an...</td>
<td>Bérost, Brenneisen, Mathieu</td>
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<td>Illicit drugs: a novel group of environmental contaminants...</td>
<td>Zuccato, Castiglioni, Bagnoli, Chiabrando, Grassi</td>
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<td>Assessment of drugs of abuse in a wastewater treatment...</td>
<td>Kumar, Tchehrane, O'Brien, Mueller, Wilkins, Padhy</td>
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<td>Mohammadzadeh, Najafi, Miladi-Gori</td>
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<td>Popp, Hammond-Weinberger, Subedi</td>
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<td>Ge, Bangs, Li, Jiang, Lat, Mueller, Thai</td>
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<td>Occurrence and fate of illicit drugs and pharmaceuticals...</td>
<td>Causeitos, Ruiz-Portugal, Ibañez, Emke, Hernandez, d...</td>
<td>The Science of the total environment</td>
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<td>Dose-dependent effects of morphine on hippocampus...</td>
<td>Mottaz, Schenberger, Fischer, Egggen, Schimmer, d...</td>
<td>Environmental pollution (Barking, Essex: 1987)</td>
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<td>Effects of voluntary exercise on the viability, proliferation...</td>
<td>Heydari, Safari, Zarabkish, Banzeghi, Miladi-Gori</td>
<td>Neuroscience Letters</td>
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<td>Genotoxic effects induced by the exposure to an...</td>
<td>Persolini, Magni, Castiglioni, Binelli</td>
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<td>Tschanké, Chen, Gerber, White</td>
<td>The Science of the total environment</td>
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Chemical Lists
##  Select List

<table>
<thead>
<tr>
<th>List Acronym</th>
<th>List Name</th>
<th>Last Updated</th>
<th>Number of Chemicals</th>
<th>List Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>HAZSUBST</td>
<td>WIKILIST: Extremely hazardous substances</td>
<td>2018-11-23</td>
<td>336</td>
<td>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)</td>
</tr>
<tr>
<td>NRTCHEMICALS</td>
<td>US National Response Team Chemical Set</td>
<td>2018-05-11</td>
<td>18</td>
<td>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.</td>
</tr>
<tr>
<td>RAPIDTOX1</td>
<td>RAPIDTOX: Test 1 Emergency Responder</td>
<td>2019-06-08</td>
<td>3988</td>
<td>Test Interface with data for emergency responders</td>
</tr>
<tr>
<td>WEBWISER</td>
<td>LIST: WEBWISER</td>
<td>2019-04-13</td>
<td>449</td>
<td>WISER is a system designed to assist emergency responders in hazardous material incidents.</td>
</tr>
</tbody>
</table>
Emergency Response List

US National Response Team Chemical Set

**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](https://www.epa.gov/cmp/national-response-team-chemical-list).

**Number of Chemicals:** 18

1 related chemical structure with this substance

- **Cyanide salts**
  - CASRN: 95-11-0
  - Mono/Mass: 0

- **VX**
  - CASRN: 5072-69-9
  - Mono/Mass: 267.142187

- **Cyclosarin**
  - CASRN: 129-99-7
  - Mono/Mass: 100.071545

- **Tabun**
  - CASRN: 77-81-6
  - Mono/Mass: 162.055615
WebWISER List

LIST: WEBWISER

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

- 2,3,7,8-Tetrachlorodibenzo-p-dioxin
  - CASRN: 576-01-6
  - DTXSID: DTXSID2021315
  - Mono. Mass: 319.9664

- 1,1,2,2-Tetrachloroethane
  - CASRN: 79-34-5
  - DTXSID: DTXSID2021310
  - Mono. Mass: 165.89061

- Tetrachloroethylene
  - CASRN: 127-18-4
  - DTXSID: DTXSID2021319
  - Mono. Mass: 163.87541

- 1,2,4,5-Tetrachlorobenzene
  - CASRN: 95-94-3
  - DTXSID: DTXSID2024320
  - Mono. Mass: 213.89061

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

Excel Download
Conclusion

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

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CCTE, US EPA Office of Research and Development, Williams.Antony@epa.gov
ORCID: https://orcid.org/0000-0002-2668-4821

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