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

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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.
Outline

• A Short History of the Dashboard
• What is the dashboard used for?
• New capabilities, data and lists
• Linkages – outbound and inbound
• Contributing to Data Quality
• Prototypes in progress
• What’s the Next Big Change?
But first

THANK YOU

TO ALL

CONTRIBUTORS
Acknowledgments upfront...

• CCTE Members
  – CompTox Chemicals Dashboard Development Team
  – Principal Investigators and postdocs
  – Curation Team

• Collaborators across the agency for data sets, testing and cross-linking

• Contributors of datasets for registration

• And you, the users for support and feedback
A SHORT HISTORY of the DASHBOARD
Earlier Dashboard Applications
Retired Dashboards – Two Gone
ToxCast and EDSP21 Dashboards

- Both dashboards served valuable purposes for a number of years but blended in now

ANNOUNCEMENT

EDSP21 and ToxCast Dashboards have been Discontinued...

As of August 2019 the EDSP21 and ToxCast dashboards are no longer available. All functionality previously available in those dashboards has been migrated to the CompTox Chemicals Dashboard and new data has been made available. Specifically, the invitroDB database has been updated to version 3.2 (ftp://newftp.epa.gov/comptox/High_Throughput_Screening_Data/InVitroDB_V3.2/), a significant update including new chemicals and assays.

For further details about accessing the data and functionality from the older dashboards in the new CompTox Chemicals Dashboard reference the "CompTox Chemicals Dashboard Functionality" PDF and links below.

<table>
<thead>
<tr>
<th>EDSP21 Dashboard</th>
<th>ToxCast Dashboard</th>
</tr>
</thead>
<tbody>
<tr>
<td>EDSP21 in the CompTox Dashboard</td>
<td>ToxCast in the CompTox Dashboard</td>
</tr>
<tr>
<td>CompTox Chemicals Dashboard Functionality</td>
<td>CompTox Chemicals Dashboard Functionality</td>
</tr>
</tbody>
</table>
The CompTox Portal – get it here
https://comptox.epa.gov/
WHAT IS THE DASHBOARD USED FOR?

(and some what’s new)
CompTox Dashboard
Chemicals

882 Thousand Chemicals

Bisphenol A

- Bisphenol A [TXS0702012]
- Bisphenol A bis(2-hydroxyethyl ether) diacylate [TXS0696691]
- Bisphenol A bis(2-hydroxyethyl ether) dimethacrylate [TXS0166992]
- Bisphenol A bis(2-hydroxypropyl) ether [TXS0651592]
- Bisphenol A carbonate polymer [TXS0652784]
- Bisphenol A diglycidyl ether [TXS0652484]
- Bisphenol A glycidyl methacrylate [TXS0704441]
- Bisphenol A propoxylate diglycidyl ether [TXS0103998]
- Bisphenol A propoxylate glycerolate diacylate [TXS04049126]
DSSTox growth – 2007 to 2020
>7000 new chemicals added

cumulative (all record)
CompTox Dashboard
Products and Use Categories
588k consumer products now in the database. Under constant curation and expansion…

### Methylparaben

**99-76-3 | DTXSID4022529**

Searched by Synonym from Valid Source.

#### Chemical Weight Fractions

<table>
<thead>
<tr>
<th>Product Name</th>
<th>Minimum Weight Fraction</th>
<th>Maximum Weight Fraction</th>
<th>Data Type</th>
<th>Source</th>
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<tbody>
<tr>
<td>114 9764 kodak ektachem calibrator kit 5-calibrator 1</td>
<td>0.00</td>
<td>1.00e-2</td>
<td>MSDS</td>
<td>SIRI</td>
</tr>
<tr>
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<tr>
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<td>1.00e-2</td>
<td>MSDS</td>
<td>SIRI</td>
</tr>
<tr>
<td>2540 gabe’s grit</td>
<td>0.00</td>
<td>5.00e-3</td>
<td>MSDS</td>
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</tr>
<tr>
<td>276300_solution_a e r pads</td>
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<tr>
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<td>MSDS</td>
<td>SIRI</td>
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<tr>
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<td>1.00e-2</td>
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<td>SIRI</td>
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<tr>
<td>846 6492 ektachem liquid performance verifier i</td>
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<td>1.00e-2</td>
<td>MSDS</td>
<td>SIRI</td>
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<tr>
<td>846 6492 kodak ektachem liquid performance verifier</td>
<td>0.00</td>
<td>1.00e-2</td>
<td>MSDS</td>
<td>SIRI</td>
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</table>
## Welcome to Factotum

<table>
<thead>
<tr>
<th>Category</th>
<th>Count</th>
</tr>
</thead>
<tbody>
<tr>
<td>Documents</td>
<td>512,150</td>
</tr>
<tr>
<td>Products</td>
<td>588,535</td>
</tr>
<tr>
<td>Extracted Chemicals</td>
<td>3.9 million</td>
</tr>
<tr>
<td>Products Linked To PUCs</td>
<td>67,206</td>
</tr>
<tr>
<td>Curated Chemical Records</td>
<td>1.9 million</td>
</tr>
<tr>
<td>Unique DTXSIDs</td>
<td>27,075</td>
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</tbody>
</table>
## The Factotum Database

**Formulation PUCs**

*General Category - Product Family - Product Type*

<table>
<thead>
<tr>
<th>Category</th>
<th>PUCs</th>
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<tbody>
<tr>
<td>Arts and crafts/Office supplies</td>
<td>3962</td>
</tr>
<tr>
<td>Cleaning products and household care</td>
<td>7917</td>
</tr>
<tr>
<td>Electronics/small appliances</td>
<td>2184</td>
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<tr>
<td>Home maintenance</td>
<td>5089</td>
</tr>
<tr>
<td>Landscape/Yard</td>
<td>1113</td>
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<tr>
<td>Personal care</td>
<td>38626</td>
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<tr>
<td>Pesticides</td>
<td>1472</td>
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<tr>
<td>Pet care</td>
<td>1076</td>
</tr>
<tr>
<td>Sports equipment</td>
<td>139</td>
</tr>
<tr>
<td>Vehicle</td>
<td>1743</td>
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</table>
CompTox Dashboard
Assays and Genes

882 Thousand Chemicals

and curating data, major updates to the batch searching functionality and access to real time predictions for both physiochemical and toxicity endpoints. A list of release notes is available for your review. We look forward to your feedback.
Growth in *invitrodb* data 2015:2020

~150 new assay endpoints

- >140 assay endpoints and >700 chemicals added
- Data re-pipelined with new fitting procedures and ~200k new curve fits released with this version
- >140 endpoints annotated to genes

<table>
<thead>
<tr>
<th>Approx Year</th>
<th>Invitrodb Version (Public)</th>
<th># assay endpoints</th>
<th>#chemicals (total)</th>
<th>#curve fits (chemical-aeid pairs)</th>
<th>#assay endpoints annotated to gene</th>
<th>#unique target genes annotated</th>
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<tbody>
<tr>
<td>2015</td>
<td>2.0</td>
<td>1192</td>
<td>9076</td>
<td>2,244,647</td>
<td>737</td>
<td>377</td>
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<tr>
<td>2018</td>
<td>3.1</td>
<td>1399</td>
<td>9214</td>
<td>3,281,340</td>
<td>1215</td>
<td>442</td>
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<td>2019</td>
<td>3.2</td>
<td>1473</td>
<td>9224</td>
<td>3,525,844</td>
<td>1255</td>
<td>443</td>
</tr>
<tr>
<td>2020</td>
<td>3.3</td>
<td>1614</td>
<td>9949</td>
<td>3,720,594</td>
<td>1398</td>
<td>492</td>
</tr>
</tbody>
</table>
SOME
EXAMPLES OF USAGE
Find me all “conazoles”
What chemicals in what use category?
“What’s in eye liner?”
Access *In Vitro* Bioactivity Data

ToxCast and Tox21

**Bisphenol A**

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

**Chemical Activity Summary**

**TOXCAST DATA**

- AC50 (uM): 5.73
- Assay Endpoint Name: OT_ER_ErA_0480
- Assay Description: 742
- Gene Symbol: ESR1
- Organism: Human
- Tissue: Kidney
- Assay Format Type: Cell-based
- Biological Process Target: Protein Stabilization
- Detection Technology: Protein-Fragment Complementation
- Analysis Direction: Positive
- Intended Target Family: Nuclear Receptor

**ASSAY DETAILS**

- Data from the assay component OT_ER_ErA_0480 was analyzed into 1 assay endpoint. This assay endpoint, OT_ER_ErA_0480, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of binding reporter, measures of receptor for gain-of-signal activity can be used to understand the binding at the pathway-level as they relate to the gene ESR1. Furthermore, this assay endpoint can be referred to as a primary readout, because the performed assay has only produced 1 assay endpoint. To generalize the intended target to other relatible targets, this assay endpoint is annotated to the 'nuclear receptor' intended target family, where the subfamily is 'steroidal'.

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**Note:** The image shows a graph with various data points and a scatter plot, indicating the bioactivity data for Bisphenol A.
Access *In Vitro* Bioactivity Data

ToxCast and Tox21
GenRA (Generalised Read-Across)

Fluconazole
86386-73-4 | DTXSID3020627
Searched by Approved Name.

Generalized Read-Across (GenRA)

Step Two: Data Gap Analysis & Generate Data Matrix

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

- Fluconazole
- Hericonazole
- Fluconazole
- Cypromazole
- Pyrascantol metabolite
- Myclobutanil
- Fenbucatazole
- Tetraconazole
- Metaconomate
- Ipronacone
- Bromocazone

# of Analogs: 10

CHR: Abdominal Cavity
CHR: Adrenal Gland
CHR: Artery (General)
CHR: Auditory Stuttle Re...
CHR: Bladder duct
CHR: Blood
CHR: Blood vessel
CHR: Body Weight
CHR: Bone
CHR: Bone Marrow
CHR: Brain
CHR: Bronchus
Related Substances
e.g. Transformation Products

Aniline
62-53-3 | DTXSID8020090
Search by DSSTox Substance Id.

Transformation Parent

C.I. Solvent Yellow 2
CASRN:640-71-7
DTXSID:DTXSID020491
TOXCAST:155/235

Transformation Parent

C.I. Acid Orange 10
CASRN:1693-15-8
DTXSID:DTXSID0021082
TOXCAST:83/429

Transformation Parent

C.I. Solvent Yellow 14
CASRN:845-07-9
DTXSID:DTXSID021133
TOXCAST:188/923

Transformation Parent

C.I. Acid Black 1, disodium salt
CASRN:1004-48-8
DTXSID:DTXSID1004415
TOXCAST:1-

Transformation Parent

C.I. Basic Orange 2
CASRN:168-82-1
DTXSID:DTXSID002459
TOXCAST:17/1285

Transformation Parent

C.I. Acid Red 108, disodium salt
CASRN:6464-74-2
DTXSID:DTXSID1041710
TOXCAST:-

Transformation Parent

C.I. Solvent Yellow 36
CASRN:2481-64-9
DTXSID:DTXSID041745
TOXCAST:111/481

Transformation Parent

C.I. Acid Yellow 11, sodium salt
CASRN:659-83-6
DTXSID:DTXSID047451
TOXCAST:36/422

Transformation Parent

C.I. Solvent Black 3
CASRN:4107-28-5
DTXSID:DTXSID10052091
TOXCAST:-

Transformation Parent

C.I. Solvent Yellow 16
CASRN:4146-14-1
DTXSID:DTXSID305208
TOXCAST:-
Related Substances for Markush
Identifiers to Support Searches

**Bisphenol A**

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

<table>
<thead>
<tr>
<th>Synonym</th>
<th>Quality</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bisphenol A</td>
<td>Valid</td>
</tr>
<tr>
<td>4,4'-Propane-2,2-diyl</td>
<td>Valid</td>
</tr>
<tr>
<td>Phenol, 4,4'-{1-methylidene}bis-</td>
<td>Valid</td>
</tr>
<tr>
<td>80-05-7</td>
<td>Valid</td>
</tr>
<tr>
<td>BPA</td>
<td>Valid</td>
</tr>
<tr>
<td>4,4'-Propane-2,2-diyl</td>
<td>Valid</td>
</tr>
<tr>
<td>Phenol, 4,4'-{1-methyl</td>
<td>Valid</td>
</tr>
<tr>
<td>4-06-00-0617</td>
<td>Beilstein Registry Number</td>
</tr>
<tr>
<td>(4,4'-Dihydroxydiphenyl)d</td>
<td>Beilstein</td>
</tr>
<tr>
<td>2,2'-Bis(4-hydroxypheny)propane</td>
<td>Good</td>
</tr>
<tr>
<td>2,2'-Bis(4-hydroxypheny)propane</td>
<td>Good</td>
</tr>
<tr>
<td>2,2'-Bis(4-hydroxypheny)propane</td>
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<tr>
<td>2,2'-Bis(4-hydroxypheny)propane</td>
<td>Good</td>
</tr>
<tr>
<td>2,2'-Bis(4-hydroxypheny)propane</td>
<td>Good</td>
</tr>
</tbody>
</table>
Abstract Sifter – PubMed Integration searching >30 million abstracts

2,3,7,8-Tetrachlorodibenzo-p-dioxin
1746-01-6 | DTXSID2021315
Searched by Expert Validated Synonym.

Abstract Sifter

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

Optionally, edit the query before retrieving. 
(“1746-01-6” OR “2,3,7,8-Tetrachlorodibenzo-p-dioxin” OR “Tetrachlorodibenzodioxin”) AND 
(cancer OR neoplasm OR carcinogen)

To find articles quickly, enter terms to sift abstracts.  
dioxin cancer mortality  
Clear Terms

<table>
<thead>
<tr>
<th>Title</th>
<th>Authors</th>
<th>Journal</th>
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</thead>
<tbody>
<tr>
<td>Cancer mortality in German male workers exposed to p...</td>
<td>Becher, Fleisch-Jarvs, Kauppinen, Kogevinas, Stei...</td>
<td>Cancer causes &amp; control</td>
</tr>
<tr>
<td>Cancer mortality in workers exposed to 2,3,7,8-tetrach...</td>
<td>Fingerhut, Halperin, Marrow, Piactelli, Honchar, Sw...</td>
<td>The New England journal of medicine</td>
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<tr>
<td>Association between dioxin and cancer incidence and m...</td>
<td>Xu, Ye, Huang, Chen, Wu, Huang, Hu, Xia, Yu</td>
<td>Scientific reports</td>
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<tr>
<td>Estimation of the cumulated exposure to polychlorinated...</td>
<td>Fleisch-Jarvs, Steindorf, Germ, Becher</td>
<td>Environmental health perspectives</td>
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<tr>
<td>Cancer mortality in workers exposed to phenox herbici...</td>
<td>Kogevinas, Becher, Bonn, Bertazzi, Buffetta, Bueno...</td>
<td>American journal of epidemiology</td>
</tr>
<tr>
<td>Exposure to polychlorinated dioxins and furans (PCDD...</td>
<td>Fleisch-Jarvs, Berger, Gurn, Manz, Nager, Watsgott...</td>
<td>American journal of epidemiology</td>
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<tr>
<td>Mortality in employees at a New Zealand agrochemical ...</td>
<td>McBride, Burns, Heribison, Humphry, Bodner, Collins</td>
<td>Occupational medicine (Oxford, England)</td>
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<tr>
<td>Thirty-four-year mortality follow-up of BAPF employees ...</td>
<td>Zober, Messnerer, Huber</td>
<td>International archives of occupational and environm...</td>
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<tr>
<td>Ten-year mortality study of the population involved in th...</td>
<td>Bertazzi, Zocchetti, Pesatori, Guercilena, Sanarico, ...</td>
<td>American journal of epidemiology</td>
</tr>
<tr>
<td>Mortality risk among workers with exposure to dioxins</td>
<td>Collins, Bodner, Aylward, Bender, Anteau, Wilken, ...</td>
<td>Occupational medicine (Oxford, England)</td>
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<tr>
<td>Plasma dioxin levels and cause-specific mortality in an...</td>
<td>Boers, Portengen, Turner, Bueno-de-Mesquita, Hee...</td>
<td>Occupational and environmental medicine</td>
</tr>
</tbody>
</table>
Mass and Formula Searches
Supporting Mass Spectrometry
Advanced Searches
Mass Based Search

Search Results
Searched by Mass: 191.131 +/- 5.0 ppm.

335 of 335 chemicals visible
"MS-Ready" structures for non-targeted high-resolution mass spectrometry screening studies

Andrew D. McEachran, Kamel Mansouri, Chris Grulke, Emma L. Schymanski, Christoph Ruttkies and Antony J. Williams

Journal of Cheminformatics 2018 10:45
https://doi.org/10.1186/s13321-018-0299-2 © The Author(s) 2018
Received: 16 May 2018 | Accepted: 21 August 2018 | Published: 30 August 2018
MS-Ready Structures

- **Nicotine**
  - Structure: ![Nicotine Structure]
  - Molecular Formula: CN1CCC[C@H]1C1=CN=CC=C1
  - CAS Number: 54-11-5
  - SMILES: 162.1157
  - logP: 0.929
  - Bioassay: yes

- **D-Nicotine**
  - Structure: ![D-Nicotine Structure]
  - Molecular Formula: CN1CCC[C@H]1C1=CN=CC=C1
  - CAS Number: 25162-00-9
  - SMILES: 162.1157
  - logP: 0.929
  - Toxicity: no
  - Exposure: yes
  - Bioassay: yes

- **Benzoic acid, 2-hydroxy, compd. with 3-[(2S)-1-methyl-2-pyrrolidinyl]pyridine (1:1)**
  - Structure: ![Benzoic acid Structure]
  - Molecular Formula: OC(=O)C1=O(C)C=CC=C1.CN1CCC[C@H]1C1=CN=CC=C1
  - CAS Number: 22083-74-5
  - SMILES: 162.1157
  - logP: 0.953
  - Toxicity: yes
  - Exposure: no
  - Bioassay: yes

- **DL-Nicotine**
  - Structure: ![DL-Nicotine Structure]
  - Molecular Formula: CN1CCC1C1=CN=CC=C1
  - CAS Number: 300.1474
  - SMILES: 162.1157
  - logP: 0.929
  - Toxicity: no
  - Exposure: yes
  - Bioassay: no

- **DL-Nicotine-d3**
  - Structure: ![DL-Nicotine-d3 Structure]
  - Molecular Formula: [2H]C([2H])([2H])N1CCC1C1=CN=CC=C1
  - CAS Number: 69980-24-1
  - SMILES: 165.1345
  - logP: 0.929
  - Toxicity: no
  - Exposure: no
  - Bioassay: no
Find me all salts of...

Silver perfluorooctanoate
335-93-3 | DTXSID00880127
Searched by DSSTox Substance Id.
Real-Time Predictions

Predictions

Select properties to predict

- Toxicological properties
  - 96 hour fathead minnow LC50
  - 48 hour D. magna LC50
  - 48 hour T. pyriformis LC50
  - Oral rat LD50
  - Bioconcentration factor
  - Developmental toxicity
  - Ames mutagenicity
  - Estrogen Receptor RBA
  - Estrogen Receptor Binding

- Physical properties
  - Normal boiling point
  - Melting point
  - Flash point
  - Vapor pressure
  - Density
  - Surface tension
  - Thermal conductivity
  - Viscosity
  - Water solubility

Calculate
# Real-Time Predictions

<table>
<thead>
<tr>
<th>Property</th>
<th>Experimental Value</th>
<th>Consensus</th>
<th>Hierarchical clustering</th>
<th>Single model</th>
<th>Group contribution</th>
<th>Nearest neighbor</th>
</tr>
</thead>
<tbody>
<tr>
<td>96 hour fathead minnow LC50</td>
<td>5.000 -Log10(mol/L) 3.057 mg/L</td>
<td>5.194 -Log10(mol/L) 1.958 mg/L</td>
<td>5.692 -Log10(mol/L) 0.783 mg/L</td>
<td>5.151 -Log10(mol/L) 2.158 mg/L</td>
<td>4.064 -Log10(mol/L) 26.414 mg/L</td>
<td></td>
</tr>
<tr>
<td>48 hour D. magna LC50</td>
<td>4.827 -Log10(mol/L) 2.553 mg/L</td>
<td>4.920 -Log10(mol/L) 2.670 mg/L</td>
<td>5.266 -Log10(mol/L) 1.657 mg/L</td>
<td>5.317 -Log10(mol/L) 1.473 mg/L</td>
<td>3.805 -Log10(mol/L) 47.846 mg/L</td>
<td></td>
</tr>
<tr>
<td>48 hour T. pyriformis IGC50</td>
<td>5.209 -Log10(mol/L) 1.892 mg/L</td>
<td>5.074 -Log10(mol/L) 2.501 mg/L</td>
<td>5.343 -Log10(mol/L) 1.387 mg/L</td>
<td></td>
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<td></td>
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<tr>
<td>Oral rat LD50</td>
<td>2.059 -Log10(mol/kg) 2689.702 mg/kg</td>
<td>2.028 -Log10(mol/kg) 2889.132 mg/kg</td>
<td>2.050 -Log10(mol/kg) 2454.135 mg/kg</td>
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<tr>
<td>Developmental toxicity</td>
<td>true</td>
<td>true</td>
<td>true</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>Ames mutagenicity</td>
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<td>false</td>
<td>false</td>
<td>false</td>
<td>false</td>
<td></td>
</tr>
<tr>
<td>Estrogen Receptor RBA</td>
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<td>false</td>
<td>false</td>
<td>false</td>
<td>false</td>
<td></td>
</tr>
<tr>
<td>Normal boiling point</td>
<td>372.1 °C</td>
<td>331.0 °C</td>
<td>479.8 °C</td>
<td>305.5 °C</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Melting point</td>
<td>133.9 °C</td>
<td>126.4 °C</td>
<td>138.6 °C</td>
<td>136.7 °C</td>
<td></td>
<td></td>
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<tr>
<td>Flash point</td>
<td>232.7 °C</td>
<td>282.4 °C</td>
<td>240.2 °C</td>
<td>175.7 °C</td>
<td></td>
<td></td>
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</tbody>
</table>
NEW CAPABILITIES, DATA AND LISTS
Watch for our news
https://comptox.epa.gov/dashboard/news_info

CompTox Chemicals Dashboard

882 Thousand Chemicals

Latest News

10th Release of the CompTox Chemicals Dashboard Now Live July 12th 2020

July 21st, 2020 at 9:32:02 PM

The 10th release of the Dashboard is now live with >7000 additional substances added to the dataset, updates to Bioactivity Data (ToxCast/Tox21), updates to the ToxVal data (under the Hazard tab), a new Safety Tab integrating the Globally Harmonized System of Classification and Labeling of Chemicals (via PubChem), over thirty new lists and a number of bug fixes. Our next release is scheduled for late Spring/Early Summer 2021, and is presently in development. It will be a full re-architecting of the entire application. Watch this space for updates. The release addresses a number of minor bugs and includes a short list of additional functionality as described in the Release Notes here.
• A detailed list of new functionality and fixes

### NEW FUNCTIONALITY

| ICD-4105 | Add new Safety Tab and load data from PubChem mapped GHS data |
| ICD-4294 | Insert Safety tab and GHS data subtab into dev database |
| ICD-4147 | CompTox Dashboard - Null Search string should Return Message "Please input search string" |
| ICD-4248 | Close QC Notes by Default when there are no notes: Open Intrinsic properties by default |
| ICD-4233 | Collapse MS-Ready and Mixtures, Components and Neutralized Forms under Linked Substances |
| ICD-4103 | Make Genra Front End handle lack of data |
| ICD-4140 | assays on EDSP21 tab would be easier to use if alpha-sorted |
| ICD-4153 | Create Redirect page for legacy Toxcast and EDSP Dashboards |
| ICD-4255 | Edit text in batch to insist on "one per row" |
| ICD-4159 | Use PIPE instead of comma to separate names in name export in Batch Search |
| ICD-4222 | Integrate Toxval_v8 into dashboard for next release |
| ICD-4234 | Switch off ToxCast and EDSP21 dashboards |
| ICD-4241 | Add Date filter to Chemical List Ag-Grid |
| ICD-4235 | Remove Google Plus from share dropdown on home page |
| ICD-4242 | Add toolbar to chemical-lists page |
| ICD-4238 | update AG-GRID to version 21.2.0 |
| ICD-4216 | Update nuxtjs version |
| ICD-4201 | Modify navigation bar |
| ICD-4017 | Change hitcall=-1 to NO CALL instead of ACTIVE or INACTIVE |
| ICD-4285 | Add "CompTox Chemicals Dashboard" to home page |
Atrazine
1912-24-9 | DTXSID9020112
Searched by DSSTox Substance Id.

GHS Data

CID 2256

Atrazine

GHS Classification

Showing 6 of 6

Pictogram(s)

- Immediate Hazard
- Health Hazard
- Environmental Hazard

Signal

- Warning

GHS Hazard Statements

- H317: May cause an allergic skin reaction [Warning, Sensitization, Skin]
- H373: Causes damage to organs through prolonged or repeated exposure [Warning, Specific target organ toxicity, repeated exposure]
- H400: Very toxic to aquatic life [Warning, Hazardous to the aquatic environment, acute hazard]
- H410: Very toxic to aquatic life with long lasting effects [Warning, Hazardous to the aquatic environment, long-term hazard]

Precautionary Statement Codes


(The corresponding statement to each P-code can be found at the GHS Classification page.)
Over 260 Lists Now Available

- Lists ranging from 3 to >62,200 chemicals
- 27 different PFAS lists – structures and non-structure lists
- Lists added to support specific programs

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>
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<tr>
<td>CECSCREEN</td>
<td>NORMAN: HBM4EU CECscreen: Screening List for Chemicals of Emerging Concern</td>
<td>2020-07-22</td>
<td>56377</td>
<td>HBM4EU CECscreen is a suspect screening list for Chemicals of Emerging Concern (CEGs) plus metadata and predicted Phase 1 metabolites</td>
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<td>ROSINS</td>
<td>List of chemicals related to Rosins</td>
<td>2020-07-21</td>
<td>872</td>
<td>Rosin is a solid form of resin obtained from pines and some other plants, mostly conifers.</td>
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<tr>
<td>PFIASDEV1</td>
<td>PFIAS/EPA PFAS chemicals without explicit structures</td>
<td>2020-07-16</td>
<td>1072</td>
<td>List of PFAS chemicals without explicit structures - polymers and other UVCB chemicals</td>
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<td>AROMATICAMINES</td>
<td>REACH: Appendix 8 lists aromatic amines associated with azocoulorants</td>
<td>2020-07-12</td>
<td>22</td>
<td>REACH Appendix 8: aromatic amines associated with azocoulorants.</td>
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<td>CPDAT</td>
<td>EPA: CPDAT, Chemical and Products Database</td>
<td>2020-07-09</td>
<td>37143</td>
<td>Chemicals contained in the EPA’s Chemical and Products Database</td>
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<tr>
<td>EPRALISTS</td>
<td>Consolidated List of Lists under EPCRA/CERCLA/CAA §112(r) (June 2019 Version)</td>
<td>2020-07-07</td>
<td>1363</td>
<td>The List of Lists is a consolidated list of chemicals subject to: Emergency Planning and Community Right-to-Know Act (EPCRA); Comprehensive Environmental Response, Compensation and Liability Act (CERCLA); and Section 112(r) of the Clean Air Act (CAA).</td>
</tr>
</tbody>
</table>
Disinfectant By-Products
82 to 619 chemicals
Consolidated List of Lists under EPCRA/CERCLA/CAA §112(r) (June 2019 Version)

Description: The List of Lists is a consolidated list of chemicals subject to: Emergency Planning and Community Right-to-Know Act (EPCRA), Comprehensive Environmental Response, Compensation and Liability Act (CERCLA), and Section 112(r) of the Clean Air Act (CAA). This is a partial mapping and under constant curation.

Number of Chemicals: 1363

1363 chemicals

- Acetamide
  CASRN: 60-35-5
  DTXSID: 0
  TOXCAST: 17/664

- Acetonitrile
  CASRN: 75-05-8
  DTXSID: 0
  TOXCAST: 0/235

- Acrolein
  CASRN: 107-03-8
  DTXSID: 0
  TOXCAST: 2/233

- Acrylamide
  CASRN: 70-61-4
  DTXSID: 0
  TOXCAST: 2/887
Curated Wikipedia

>12,000 chemicals
Wikipedia serves the “snippet”

**Sarin**

107-44-8 | DTXSID0042371

Searched by DSSTox Substance Id.

![Sarin molecule](image)

**Wikipedia**

Sarin (NATO designation GB [short for G-series, "B"]) is an extremely toxic synthetic organophosphorus compound. A colourless, odourless liquid, it is used as a chemical weapon due to its extreme potency as a nerve agent. Exposure is lethal even at very low concentrations, where death can occur within one-to-ten minutes after direct inhalation of a lethal dose, due to suffocation from lung muscle paralysis. Unless antidotes are quickly administered.

...  

Read more

**Quality Control Notes**

**Intrinsic Properties**

- **Molecular Formula**: C₄H₁₀FO₂P
- **Average Mass**: 140.094 g/mol
- **Monoisotopic Mass**: 140.040245 g/mol
Other Lists of Interest

- Storage Tanks – Above Ground/Underground
- IRIS Chemicals refreshed to >600 chemicals
- Azo dyes (decompose to aromatic amines)
- Curated CASMI (Critical Assessment of Small Molecule Identification) datasets

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Published online 2020 Jun 23. doi: [10.3390/metabo10060260](https://doi.org/10.3390/metabo10060260)

**Revisiting Five Years of CASMI Contests with EPA Identification Tools**

Andrew D. McEachran, Alex Chao, Hussein Al-Ghoul, Charles Lowe, Christopher Gruke, Jon R. Sobus, and Antony J. Williams.
Lists provide a landscape overview

### Presence in Lists

#### Federal
- TOXCASST_Phase1 - EPA ToxCast Screening Library (Phase I Subset)
- TOXCASST_PhaseII - EPA ToxCast Screening Library (Phase II Subset)
- TOXCAST_ph2 - EPA ToxCast Screening Library (ph2 Subset)
- CHEMINV: EPA Chemical Inventory for ToxCast
- TOXCAST: EPA ToxCast Screening Library
- ENDOCRINE: EDSP Universe of Chemicals
- ECOTOX: Ecotoxicology knowledgebase
- WATER: EPA: Chemicals in hydraulic fracturing (fluids Table H-2)
- WATER: EPA: Chemicals associated with hydraulic fracturing
- EPA: Consumer Products Suspect Screening Result
- TOXCAST: EPA ToxCast Screening Assay In Vitro DB Version 3
- EPA: High Production Volume List
- CHEMINV: ToxCast/Tox21 Chemical inventory available as DMSO solutions (20181123)
- TOX21SL: Tox21 Screening Library
- LIST: Substances Added to Food (formerly EAFUS)
- TSCA Active Inventory non-confidential portion (updated March 20th 2020).

#### US State
- None.

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

#### Other
- COSMOS DB cosmetics database
- NORMAN: REACH Chemicals List provided to NORMAN Network
- NORMAN: Norman Network Suspect Screening List (USDAT)
- EPA: CPDAT, Chemical and Products Database
- Global harmonization system aggregated chemical data list (skin and eyes)
- MASSSPECDB: Thermo's mzCloud Database
- NORMAN: Combined 2000/2006 EU Cosmetic Ingredients Inventory
- WATER: STOFF-IDENT Database of Water-Related Substances
- ESTROGEN: Integrated pathway model for the Estrogen Receptor
- NEURO: DNT Screening Library
- PESTICIDES|EPA: Pesticide Chemical Search Database
- ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (COMPARA)
- LIST: Wikipedia chemicals
- LIST: Hazardous Substances Data Bank
- PESTICIDES|EPA: List of Inert Ingredients Food and Nonfood Use UPDATED 10/25/2019
Potential Use Cases

- Batch search a list of chemicals to identify presence in >280 lists
## Cross-walking lists of interest

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<th>D</th>
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Are there azo dye mass spectra?

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### Azo dyes listed in “water” lists

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<td>DTXSID3020201</td>
<td>C.I. Direct Brown 85</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>DTXSID9020324</td>
<td>Chocolate Brown HT</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>DTXSID502491</td>
<td>4-(Dimethylamino)az</td>
<td>Y</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>DTXSID6020511</td>
<td>3,3'-Dimethylbenzidine</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>DTXSID6021087</td>
<td>C.I. Acid Orange 10</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
LINKAGES
OUTBOUND and INBOUND
Increasingly important identifier

The DTXSID

Atrazine
1912-24-9 DTXSID9020112

Wikipedia

Atrazine is a herbicide of the triazine class. It is used to prevent pre-emergence broadleaf weeds in crops such as maize (corn) and sugarcane and on turf such as golf courses and residential lawns. Atrazine's primary manufacturer is Syngenta and it is one of the most widely used herbicides in US and Australian agriculture.
As of 2001, atrazine was the most commonly detected pesticide contaminating drinking water in the United States. Studies suggest it is an endocrine disruptor.
Read more

Quality Control Notes

Intrinsic Properties

- Molecular Formula: C_{9}H_{12}ClN_{5}
- Average Mass: 215.69 g/mol
- Monoisotopic Mass: 215.093773 g/mol

Structural Identifiers

- IUPAC Name: 6-Chloro-N-2-ethyl-N-4-(propan-2-yl)-1,3,5-triazine-2,4-diamine
- SMILES: CC(N=C(N(C(Cl)=NCl)=N1)
In-links from various sources

- Wikipedia
- AOP Wiki
- PubChem
- MassBank
- UniChem
The DTXSID Identifier

Wikidata:Property proposal/DTXSID

< Wikidata:Property proposal

DSSTOX substance identifier  [ edit ]

Originally proposed at Wikidata:Property proposal/Natural science

Done: DSSTox substance ID (P3117) (Talk and documentation)

<table>
<thead>
<tr>
<th>Description</th>
<th>The DTXSID is the DSSTox substance identifier used in the Environmental Protection Agency CompTox Dashboard.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data type</td>
<td>External identifier</td>
</tr>
<tr>
<td>Domain</td>
<td>chemical substance (Q7529)</td>
</tr>
<tr>
<td>Example</td>
<td>benzene (Q2270) → DTXSID3039242 [i]</td>
</tr>
<tr>
<td>Planned use</td>
<td>Adding DTXSIDs to @wikidata using a bot or possible Mix&amp;Match, based on InChIKey matches and this CCZero data on Figshare: <a href="https://figshare.com/articles/Mapping_file_of_InChiStrings_InChiKeys_and_DTXSIDs_for_the_EPA_CompTox_Dashboard/3578313/1">https://figshare.com/articles/Mapping_file_of_InChiStrings_InChiKeys_and_DTXSIDs_for_the_EPA_CompTox_Dashboard/3578313/1</a> [i] .</td>
</tr>
<tr>
<td>Formatter URL</td>
<td><a href="https://comptox.epa.gov/dashboard/$1">https://comptox.epa.gov/dashboard/$1</a></td>
</tr>
</tbody>
</table>

Motivation

The Environmental Protection Agency (Q16919823)’s CompTox Dashboard is a fairly new website, but the DSSTox project exists for much longer (Distributed structure-searchable toxicity (DSSTox) public database network: a proposal (Q26701365)). The Dashboard aggregates over 720 thousand chemical substances and is open data. The CompTox dashboard also provides access to synonyms, experimental and predicted property data, product and functional use details and EPA’s Toxcast Bioassay data. The DTXSIDs are unique substance identifiers, already been included into PubChem and the EBI UniChem InChIKey mapping files. The DTXSIDs will also be included into the BridgeDb metabolite mapping databases on short notice. Egon Willighagen (talk) 17:48, 24 August 2016 (UTC)
Increasing number of outlinks

- External Links reduce time to discovery

### Acrylamide

**Identification:** 79-06-1 | DTXSID5020027

**Acrylamide** is a chemical compound with the molecular formula C₃H₅N₂O. It is a colorless liquid with a strong, characteristic odor. Acrylamide is widely used in the production of acrylic fibers, resins, and polymers, as well as in the synthesis of other organic compounds. It is also used in the treatment of lung cancer and in the production of rubber and plastics.

#### General
- **EPA Substance Registry Service**
- **Household Products Database**
- **Chemical Entities of Biological Interest (ChEBI)**
- **PubChem**
- **ChemSpider**
- **CPCat**
- **DrugBank**
- **HMDB**
- **Wikipedia**
- **MSDS Lookup**
- **CheMBL**
- **Chemical Vendors**
- **CAS-DEHHA**
- **NIOSH Chemical Safety Cards**
- **ToxPlanet**
- **ACS Reagent Chemicals**
- **WikiData**
- **ChemHat: Hazards and Alternatives Toolbox**

#### Toxicology
- **ACToR**
- **DrugPortal**
- **CCPR**
- **ChemView**
- **CTD**
- **ChemPortal**
- **Gene-Tox**
- **HSDB**
- **ToxCast Dashboard 2.0**
- **LactMed**
- **International Toxicity Estimates for Risk**
- **ATSDR Toxic Substances Portal**
- **Superfund Chemical Data matrix**
- **NIOSH IDLH Values**
- **ACToR PDF Report**
- **Toxics Release Inventory**
- **CREST**
- **National Air Toxics Assessment**
- **Superfund Chemical Data matrix**

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

#### Analytical
- **FOR-IDENT**
- **NEMIS: National Environmental Methods Index**
- **RSC Analytical Abstracts**
- **Tox21 Analytical Data**
- **MONA: MassBank North America**
- **m2Cloud**
- **NIST: NIST IR Spectrum**
- **NIST MS Spectrum**
- **ECOTOX**
- **MassBank**
- **NEMIS: National Environmental Methods Index**
- **NIST: NIST Antoine Constants**
- **IR Spectra on PubChem**
- **NIST: NIST Kovats Index values**
- **Protein DataBank**
New Outlinks of Interest
State-Specific Water Quality Standards

State-Specific Water Quality Standards Effective under the Clean Water Act (CWA)

EPA has compiled state, territorial, and authorized tribal water quality standards that EPA has approved or are otherwise in effect for Clean Water Act purposes. This compilation is continuously updated as EPA approves new or revised WQS.

In instances when state-specific water quality standards have not been developed or approved by EPA, the Agency will propose and/or promulgate standards for a state until such time as the state submits and EPA approves their own standards. Any federally-proposed or promulgated replacement water quality standards are also identified.

Please note the water quality standards may contain additional provisions outside the scope of the Clean Water Act, its implementing federal regulations, or EPA’s authority. In some cases, these additional provisions have been included as supplementary information.

EPA is posting the water quality standards as a convenience to users and has made a reasonable effort to assure their accuracy. Additionally, EPA has made a reasonable effort to identify parts of the standards that are approved, disapproved, or are otherwise not in effect for Clean Water Act purposes.

- See EPA’s ComTox Chemical Dashboard for more information on this chemical.

<table>
<thead>
<tr>
<th>State</th>
<th>Parameter (the name used by the state)</th>
<th>Application</th>
<th>Criteria Magnitude</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alaska</td>
<td>atrazine</td>
<td>drinking water MCL, (water supply (drinking, culinary and food processing); contact recreation) (Human Health)</td>
<td>0.0030 mg/l</td>
</tr>
<tr>
<td>Arizona</td>
<td>atrazine</td>
<td>Domestic Water Source (DWS) (Human Health)</td>
<td>3 μg/l</td>
</tr>
<tr>
<td>Arizona</td>
<td>atrazine</td>
<td>Full-Body Contact (FBC) (Human Health)</td>
<td>32667 μg/l</td>
</tr>
<tr>
<td>Arizona</td>
<td>atrazine</td>
<td>Partial-Body Contact (PBC) (Human Health)</td>
<td>32667 μg/l</td>
</tr>
<tr>
<td>California Region 1 - North Coast</td>
<td>atrazine</td>
<td>municipal or domestic supply (Human Health)</td>
<td>0.0030 mg/l</td>
</tr>
<tr>
<td>California Region 2 - San Francisco Bay</td>
<td>atrazine</td>
<td>municipal supply</td>
<td>0.0030 mg/l</td>
</tr>
<tr>
<td>California Region 2 - Central Coast</td>
<td>atrazine</td>
<td>domestic or municipal supply</td>
<td>0.0030 mg/l</td>
</tr>
<tr>
<td>California Region 4 - Los Angeles</td>
<td>atrazine</td>
<td>municipal and domestic water supply (Human Health)</td>
<td>0.001 mg/l</td>
</tr>
<tr>
<td>California Region 9 - San Diego</td>
<td>atrazine</td>
<td>municipal or domestic supply (Human Health)</td>
<td>0.0030 mg/l</td>
</tr>
<tr>
<td>Colorado</td>
<td>atrazine</td>
<td>drinking water supply (Human Health)</td>
<td>3 μg/l</td>
</tr>
</tbody>
</table>
### Atrazine

#### Chemical Vendors

<table>
<thead>
<tr>
<th>Vendor</th>
<th>PubChem SID</th>
<th>Purchasable Chemical</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Yuha Chemical</strong></td>
<td>355047054</td>
<td>LT4922</td>
</tr>
<tr>
<td></td>
<td>347737622</td>
<td>LT6957</td>
</tr>
<tr>
<td><strong>Achemo Scientific Limited</strong></td>
<td>252453703</td>
<td>AC-11427</td>
</tr>
<tr>
<td><strong>Sigma-Aldrich</strong></td>
<td>329753681</td>
<td>31212_SIAL</td>
</tr>
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<td></td>
<td>329756651</td>
<td>45330_SIGMA</td>
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<tr>
<td></td>
<td>24871790</td>
<td>48187_SUPELCO</td>
</tr>
<tr>
<td></td>
<td>24872608</td>
<td>49085_SUPELCO</td>
</tr>
<tr>
<td></td>
<td>329769969</td>
<td>90935_SIAL</td>
</tr>
<tr>
<td></td>
<td>329823655</td>
<td>PS380-250MG_SUPELCO</td>
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<tr>
<td></td>
<td>24899206</td>
<td>PS380_SUPELCO</td>
</tr>
<tr>
<td><strong>ZINC</strong></td>
<td>256808431</td>
<td>ZINC3078958</td>
</tr>
<tr>
<td><strong>Acadechem</strong></td>
<td>321908354</td>
<td>ACDS-021206</td>
</tr>
</tbody>
</table>
Atrazine

CAS Number
1912-24-9

Synonym(s)
Aatrex; Akticon; Argezin; Atranex; Atrataf; Atrazin; Atred; Atrex; Candex; Chromozin; Cyazin; Farmaco atrazine; Fenamine; Gesaprim; Inakor; Caswell No. 063; Oleogesaprim; Pitezin; Primatol; Primaze; Radazin; Strazine; Vectal; Weedex A; Wonuk; Zeapos; Zeazin; Zeazine; EPA Pesticide Code: 080803
CONTRIBUTING to DATA QUALITY
Ongoing Data Review
Thanks to our curators!

Cumulative Manual

Cumulative Manual
Data Curation Level

- View the level of curation for any chemical
- If you see any issues let us know
As users, please **contribute**

- **We welcome your comments:**
  https://comptox.epa.gov/dashboard/contact_us

   We welcome feedback regarding your experiences using the CompTox Chemicals Dashboard. Please send us your comments and questions using the form below.

   williams.antony@epa.gov

   Please add list of disinfectants

   It would be useful to add the chemicals associated with EPA's "List N: Disinfectants for Use Against SARS-CoV-2 (COVID-19)" available at: https://www.epa.gov/pesticide-registration/list-n-disinfectants-use-against-sars-cov-2-covid-19

   I'm not a robot

   reCAPTCHA

   Privacy - Terms

   Back  Send
Please help curate the data...

• Users can identify issues with all of our data
  – Suggest chemicals to add to lists
  – Suggest related substances – e.g. metabolites, degradants
  – Flag errors in the data – e.g. properties

• We are now receiving daily feedback – “Submit Comment”
Submit Comments
We will provide feedback…

New Comment

Details to be submitted with your comment

Text selected: Danish_EPA_SCPFAS_Report_2015
Found On: July 22nd 2020, 8:25:09 pm
Original Query: /dsstoxdb/results?search=PFOS#properties
Browser: Chrome 84

Comment

There appears to be a value missing associated with the “Danish_EPA_SCPFAS_Report_2015”. Maybe worth checking if there should be a value added?

Email address

williams.antony@epa.gov

I'm not a robot

Submit
## Crowdsourced Comments

### Chemical

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Structure</th>
<th>Date</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxazole, 2-ethyl-4,5-dimethyl-</td>
<td><img src="image" alt="Structure" /></td>
<td>2020-07-22</td>
<td>4,5-Dimethyl-2-ethyloxazole is just a BAD name - remove? Add 2-Ethyl-4,5-dimethyloxazole WLN is T5N COJ B2 D1 E1 REAXYS/BRN is S07360 FEMA 3672 MFCDD0036664 Barrie</td>
</tr>
<tr>
<td>4-Decenoic acid, ethyl ester, (4E)-</td>
<td><img src="image" alt="Structure" /></td>
<td>2020-07-22</td>
<td>Add names Ethyl (4E)-4-decenoate (uninverted CAS name) Ethyl (E)-dec-4-enolate (IUPAC) FEMA 3642 REAXYS/BRN 1770966 WLN 6U3VO2 &amp;&amp;E or trans Form REACH 278-509-4 (ex EINECS) PubChem CID 5362583 MFCDD0015574 UNII-3189X5937N Barrie</td>
</tr>
<tr>
<td>Hexanedioic acid, diisononyl ester</td>
<td><img src="image" alt="Structure" /></td>
<td>2020-07-21</td>
<td>the tox cast curves for some chemicals will not display, specifically the toxcast/tox21 tab is missing from the left side menu on the dashboard. You can only display the toxcast summary (that shows there are results from toxcast/tox21) or the toxcast models. Examples are 33703-08-1 and 27176-16-1.</td>
</tr>
<tr>
<td>2-Pentenal, 5-[(methylthio)-2-[(methylthio)methyl]-</td>
<td><img src="image" alt="Structure" /></td>
<td>2020-07-20</td>
<td>2,8-Dithianon-4-en-4-carboxaldehyde should be.aldheyde 2-Methylthiomyethyl-5-methylthiopent-2-enal BAD name - remove, on corrected as below 5-(Methylthio)-2-(methylthio)methylpent-2-en-1-al 5-(Methylthio)-2-(methylthio)methylpent-2-enal known trivially as Methialdo REAXYS/BRN is 2241044 WLN is 153UYV15151 Barrie</td>
</tr>
<tr>
<td>Dipentyl 2-hydroxybutanedioate</td>
<td><img src="image" alt="Structure" /></td>
<td>2020-07-20</td>
<td>well known as Dipentyl malate WLN SOYQ1VOS Barrie</td>
</tr>
<tr>
<td>Tricyclo[1.1.0.0-2,4]tetraphosphate</td>
<td><img src="image" alt="Structure" /></td>
<td>2020-07-20</td>
<td>This comment or question is asked of me somewhat frequently, is DTXSID1024382 white phosphorus as it is listed as a synonym, or is it more appropriate to say DTXSID90923991 is white phosphorus? Any clarification that could be provided on DTXSID90923991’s entry on the Dashboard would be appreciated.</td>
</tr>
</tbody>
</table>
PROTOTYPES in PROGRESS
Proof-of-Concept: Structure/Substructure/Similarity Searches
Other Prototypes in Progress

- “Structure Standardization” services to produce MS-Ready and QSAR-ready data
- Single predictions already available. Batch predictions in development.
“RapidTox” Proof-of-Concept
RapidTox Dashboard

Decision-support tool to integrate chemistry, toxicity and exposure information

Under different federal statutes, EPA makes a broad range of decisions to protect public health and the environment from unintended consequences of using chemicals. Decisions about chemicals are also made by other Federal Agencies, State Environmental and Health Agencies, International Governmental Agencies and Industry. As examples, there are specific federal laws for pesticides, drinking water contaminants, commercial and industrial chemicals, chemicals found on contaminated sites and endocrine disrupting chemicals.

These laws give EPA the authority to gather health, safety and exposure data on chemicals, require necessary testing, and control human and environmental exposures. EPA’s computational toxicology researchers are integrating available chemical information including chemistry, toxicity and exposure information into an online tool called RapidTox to help decision-makers quickly and efficiently evaluate chemicals. To help decision-makers leverage this information effectively, researchers are now customizing this tool to help EPA and states meet the requirements under various federal statutes as well as state and local laws.
An automated framework for compiling and integrating chemical hazard data

Leora Vegosen¹,² · Todd M. Martin²

Received: 3 October 2019 / Accepted: 13 December 2019 / Published online: 21 January 2020
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Now: “Hazard Comparison Dashboard”

- **Watch this space…**
WHAT’S THE NEXT BIG CHANGE?
First - An Announcement

• After 5 years & 10 releases, we have reached the end of *this* technology architecture
• The dashboard: a prototype that kept growing
• We are starting *afresh* with a new architecture based on a datahub and new user experience
• First release scheduled for March 2021
  – migration of existing capabilities
  – supporting increased frequency of data releases
  – existing dashboard will remain online for smooth transition
Short Term Goals for Release

• Using new table widgets to unify tabulated data handling across the application
• Rebuilding visualization widgets to support multiple applications
• Service-based architecture will ultimately provide **public API** to access datahub
• Faster, more flexible searching
Future Integration Planned…
The ACToR Database
The CompTox Chemistry Dashboard: a community data resource for environmental chemistry

Antony J. Williams¹,*, Christopher M. Grulke¹, Jeff Edwards¹, Andrew D. McEachran², Kamel Mansouri¹,²,⁴, Nancy C. Baker³, Grace Patlewicz¹, Imran Shah¹, John F. Wambaugh¹, Richard S. Judson¹ and Ann M. Richard¹
• We owe a great debt to the curators who have invested efforts over ~20 years
Downloadable Data Will Be Updated

Downloads

DSSTox Identifier to PubChem Identifier Mapping File

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

SID | CID | DTXSID
--- | --- | ---
316388891 | 20404 | DTXSID30873143
316388890 | 10142816 | DTXSID70873142
316388889 | 50742127 | DTXSID40873139
316388888 | 19073841 | DTXSID20873137
316388887 | 11505215 | DTXSID00873135
316388886 | 25021861 | DTXSID80873133
316388885 | 2784427 | DTXSID00873131
316388884 | 6731 | DTXSID00873130

DSSTox identifiers mapped to CAS Numbers and Names File

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

<table>
<thead>
<tr>
<th>casrn</th>
<th>dssstox_substance_id</th>
<th>preferred_name</th>
</tr>
</thead>
<tbody>
<tr>
<td>26148-68-5</td>
<td>DTXSID7020001</td>
<td>Ace-alpha-C</td>
</tr>
<tr>
<td>107-29-9</td>
<td>DTXSID7020004</td>
<td>Acetone1oxide</td>
</tr>
<tr>
<td>60-35-1</td>
<td>DTXSID7020005</td>
<td>Acetamide</td>
</tr>
<tr>
<td>103-99-2</td>
<td>DTXSID7020006</td>
<td>Acetaminophen</td>
</tr>
<tr>
<td>968-81-0</td>
<td>DTXSID7020007</td>
<td>Acetohexamide</td>
</tr>
<tr>
<td>18523-69-8</td>
<td>DTXSID7020008</td>
<td>Acetomaldehyde(4-(5-nitro-2-furyl)-2-thiazoly) hydrazone</td>
</tr>
<tr>
<td>75-05-8</td>
<td>DTXSID7020009</td>
<td>Acetone</td>
</tr>
<tr>
<td>127-96-9</td>
<td>DTXSID6020010</td>
<td>Acetolene</td>
</tr>
<tr>
<td>215734-38-5</td>
<td>DTXSID6020012</td>
<td>N'-Acetyl-4-(hydroxymethyl) phenylhydrazine</td>
</tr>
</tbody>
</table>
Conclusion

• The Dashboard is our primary web-based tool for delivering data to the community.

• Data growth continues unabated – new chemicals, toxicity data, products, predictions, *in vitro* data…

• Data curation is a **critical** aspect of the project.

• Proof-of-concept applications in development:
  – Structure standardization (MS-Ready/QSAR-Ready)
  – Structure-substructure-similarity searching
  – Hazard Comparison Dashboard and RapidTox workflows

• Next release (March 2021) will be a full **rebuild** of the architecture. Public API in development.
Antony Williams
US EPA Office of Research and Development
National Center for Computational Toxicology (NCCT)
Williams.Antony@epa.gov
ORCID: https://orcid.org/0000-0002-2668-4821

(Please note I am one small cog in the engine that makes the dashboard happen...)