

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

Antony Williams

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

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

*July 23rd 2020
Communities of Practice*

- 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***

- **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

ACToR Home Data Collections Search Assays Chemical Download Apps

Bisphenol A
80-05-7 | DTXSID7020182

INChI: InChI=1S/C15H16O2=15O2,11-3-7-13|168-41(1)12-5-8-14(17)10-6-12h3-10,16-17H,1-2H3
INChI Key: HSBACLAFKNSITLJHFFFDYJSA-N
SMILES: CC(C)(C1=CC=C(O)C=C1)C(C)(C)C2=CC=C(O)C=C2
Molecular Formula: C15H16O2
Molecular Weight: 228.291 g/mol

Synonyms

Hazard

Show Data **HSIA Data**

- Chemicals known to the State of California to Cause Cancer or Reproductive Toxicity (Prop 65) (2014)
- ChemIST combination of 2 Data from: and Propyls 601
- ChemIST combination of files from EU Research lab
- ChemIST combination of files from Metabo Validator Group
- CPDS Report on Carcinogenic Potency URL (URL: CAL: Benzene)
- OSDTA Cancer Potency Database Summary
- OSDTA Cancer Potency Database URL
- OSDTA NCTR Estrogen Receptor Database
- OSDTA NTP B2 GenTox Index
- OSDTA NTP B2i Chronic/ Cancer Study Index
- OSDTA NTP B2i Chronic/ Cancer Study Index
- OSDTA NTP B2i GenTox Index
- OSDTA NTP B2i GenTox Index
- OSDTA IRD Study Summaries
- OSDTA IRD URL

EPA iCSS ToxCast Dashboard Home Export

Choose a view: Assays Chemicals Database: prof_dashboard_v2 Dashboard: v2

Chemicals - 1

CASRN	Chemical Name
80-05-7	Bisphenol A

Assays - 1001

Assay Endpoint Name: Gene Symbol:

Active - MG Only All Tested

Assay Component	Endpoint Name	Gene Symbol
ACEA_T4TD_S0hr_Negative		
ACEA_T4TD_S0hr_Positive		
APR_HepG2_CellCycloArrest_Th_0h		
APR_HepG2_CellCycloArrest_Th_1up		
APR_HepG2_CellLoss_Th_0h		
APR_HepG2_CellLoss_Th_1up		
APR_HepG2_MitoSubstCSP_Th_0h		
APR_HepG2_MitoSubstCSP_Th_1up		
APR_HepG2_MitoMembPot_Th_0h		
APR_HepG2_MitoMembPot_Th_1up		
APR_HepG2_MitoMembPot_Th_0h		
APR_HepG2_MitoMembPot_Th_1up		
APR_HepG2_MitoMembPot_Th_0h		
APR_HepG2_MitoMembPot_Th_1up		
APR_HepG2_MitoMembPot_Th_0h		
APR_HepG2_MitoMembPot_Th_1up		
APR_HepG2_MitoMembPot_Th_0h		
APR_HepG2_MitoMembPot_Th_1up		
APR_HepG2_MitoMembPot_Th_0h		
APR_HepG2_MitoMembPot_Th_1up		

Chemical Activity Summary

Active endpoints for 80-05-7

Sorted response is calculated by dividing the response values by the activity cutoff enabling response comparison across assay endpoints.

EPA United States Environmental Protection Agency

CPCat: Chemical and Product Categories Contact Us

You are here: EPA Home > Computational Toxicology Research > Chemical Use

Home Search Results Dictionary Download Help

Chemical: BISPENOLA CASRN: 80-05-7

Export Use Data Export Product Data

Use Information:

CPCat Description	Source Description	ACToR Data Set/List	Source	Class of Chemical Category
consumer_use_ACToRUseDB	Consumer Use		ACToR UseDB	Use Categories
personal_care_ACToRUseDB	Personal Care Product		ACToR UseDB	Use Categories
industrial_manufacturing_ACToRUseDB	Chemical Industrial		ACToR UseDB	Use Categories
child_use_detected	Consumer Products	The Danish EPA Exposure of 2-year-olds to chemical substances in Consumer Products. This project included a survey of the products as well as chemical analyses and risk assessments of a number of selected products that 2-year-old children come into contact with	ACToR Data Sets and Lists	Use Categories

EPA United States Environmental Protection Agency

EDSP21 Dashboard Endocrine Disruptor Screening Program for the 21st Century

Chemical Summary Public Information Bioactivity Summary Bioactivity High-Throughput Exposure Assay Definitions Dictionary

EDSP Dashboard Overview

EDSP Dashboard Overview

Congress requires EPA's Endocrine Disruptor Screening Program to evaluate chemicals for potential endocrine disruption, and there are thousands of chemicals of interest to the program. EPA researchers developed the Endocrine Disruptor Screening Program for the 21st Century Dashboard (EDSP21 Dashboard) to provide access to new chemical data on over 1,000 chemicals of interest.

The purpose of the EDSP21 Dashboard is to help the Endocrine Disruptor Screening Program evaluate chemicals for endocrine-related activity.

The data for this version of the Dashboard comes from various sources -

- Rapid, automated (or in vitro high-throughput) chemical screening data generated by the EPA's Toxicity Forecaster (ToxCast) project and the federal Toxicity Testing in the 21st Century (Tox21) collaboration.
- Chemical exposure data and prediction modes (EpopCastDB).
- High quality chemical structures and annotations (GGSTox).
- PhysChem Properties Database (PhysChemDB).

ToxCast Data Use Considerations

- The activity of a chemical in a specific assay does not necessarily mean that it will cause toxicity or an adverse health outcome. There are many factors that determine whether a chemical will cause a specific adverse health outcome. Careful review is required to determine the use of the data in a particular decision context.
- Interpretation of ToxCast data is expected to change over time as both the science and analytical methods improve.

EPA will continuously add functionality and improve overall usability and performance.

To get the best possible experience using the EDSP Dashboard application we recommend using Mozilla Firefox or Google Chrome.

Retired Dashboards – Two Gone



**CompTox
Chemicals
Dashboard**



**Aggregated
Publicly Available
Chemical Data
ACToR**



**ToxCast
Dashboard
High-throughput
screening data**



EDSP21 Dashboard
High-throughput screening
and exposure estimates for
evaluating chemicals for
potential endocrine activity



RapidTox
Decision support workflows
to integrate chemistry,
toxicity, and exposure
information



Downloadable Data

- 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.

EDSP21 Dashboard

[EDSP21 in the CompTox Dashboard](#)

 [CompTox Chemicals Dashboard Functionality](#)

ToxCast Dashboard

[ToxCast in the CompTox Dashboard](#)

 [CompTox Chemicals Dashboard Functionality](#)

The CompTox Portal – get it here <https://comptox.epa.gov/>



**CompTox
Chemicals
Dashboard**



**Aggregated
Publicly Available
Chemical Data
ACToR**



**ToxCast
Dashboard
High-throughput
screening data**



EDSP21 Dashboard
High-throughput screening
and exposure estimates for
evaluating chemicals for
potential endocrine activity



RapidTox
Decision support workflows
to integrate chemistry,
toxicity, and exposure
information



Downloadable Data

CompTox Chemicals Dashboard

https://comptox.epa.gov/dashboard



EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

875 Thousand Chemicals

Chemicals Product/Use Categories Assay/Gene

SEARCH

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey

Identifier substring search

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

BATCH SEARCH

Step Four: Select Data Output Format and Choose Data Fields to Download

Select Input Type(s):
Identifiers
Chemical Name
CASRN
InChIKey
EPA Substance
DSCSA Compound
InChIKey Sequence
MS-Ready Formula
EPA Formula
Monoisotopic Mass
Display All Chemicals Download Chemical Data

Select Output Format:
Excel Download

Customize Results:
Select All in Lists
Chemical Identifiers
CASRN
Chemical Name
InChIKey

Previews in Lists:
Pharmaceutical from DTXSID
ACQF655 Extremely Hazardous Substance List and Threshold Planning Quantities
AQSII Acute Exposure Guideline Levels
Amphibole Minerals
ANERGEM Androgen Receptor Chemicals

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

TOX DATA

Bisphenol A
80-05-7 | DTXSID7020182
Searched by Expert Validated Synonym.

Hazard

Download Columns

Max	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Substance	Source
MES	Short-term	Critical Air	short-term	500	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOO
MES	Short-term	Marginal Air	short-term	100	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOO
MES	Short-term	Negligible Air	short-term	15	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOO
MES	Soil	Negligible Soil	chronic	100000	mg/kg	-	soil	-	TG 230 Military Exposure Guidelines Table	DOO
MES	Long-term	Soil Negligible Water	chronic	7	mg/L	-	oral	-	TG 230 Military Exposure Guidelines Table	DOO

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

BATCH SEARCH

Step Three: Run GenRA Prediction

Neighbors by: Chem Morgan Filter by: InChI Data

Summary Data Gap Analysis

Neighbors by: Chem Morgan	Filter by: InChI Data	Summary Data Gap Analysis
4-ethylphenol	4-ethylphenol	4-ethylphenol
4-isobutylphenol	4-isobutylphenol	4-isobutylphenol
4-nonylphenol	4-nonylphenol	4-nonylphenol
4-tert-butylphenol	4-tert-butylphenol	4-tert-butylphenol
4-vinylphenol	4-vinylphenol	4-vinylphenol
4-propylphenol	4-propylphenol	4-propylphenol
4-cyclohexylphenol	4-cyclohexylphenol	4-cyclohexylphenol
4-phenylphenol	4-phenylphenol	4-phenylphenol
4-ethylphenol	4-ethylphenol	4-ethylphenol
4-isobutylphenol	4-isobutylphenol	4-isobutylphenol
4-nonylphenol	4-nonylphenol	4-nonylphenol
4-tert-butylphenol	4-tert-butylphenol	4-tert-butylphenol
4-vinylphenol	4-vinylphenol	4-vinylphenol
4-propylphenol	4-propylphenol	4-propylphenol
4-cyclohexylphenol	4-cyclohexylphenol	4-cyclohexylphenol
4-phenylphenol	4-phenylphenol	4-phenylphenol

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

BIOACTIVITY

Bisphenol A
80-05-7 | DTXSID7020182
Searched by Expert Validated Synonym.

Chemical Activity Summary

TOXCAST DATA

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

SIMILARITY

Bisphenol A
80-05-7 | DTXSID7020182
Searched by Expert Validated Synonym.

Searched with a similarity threshold of 0.8

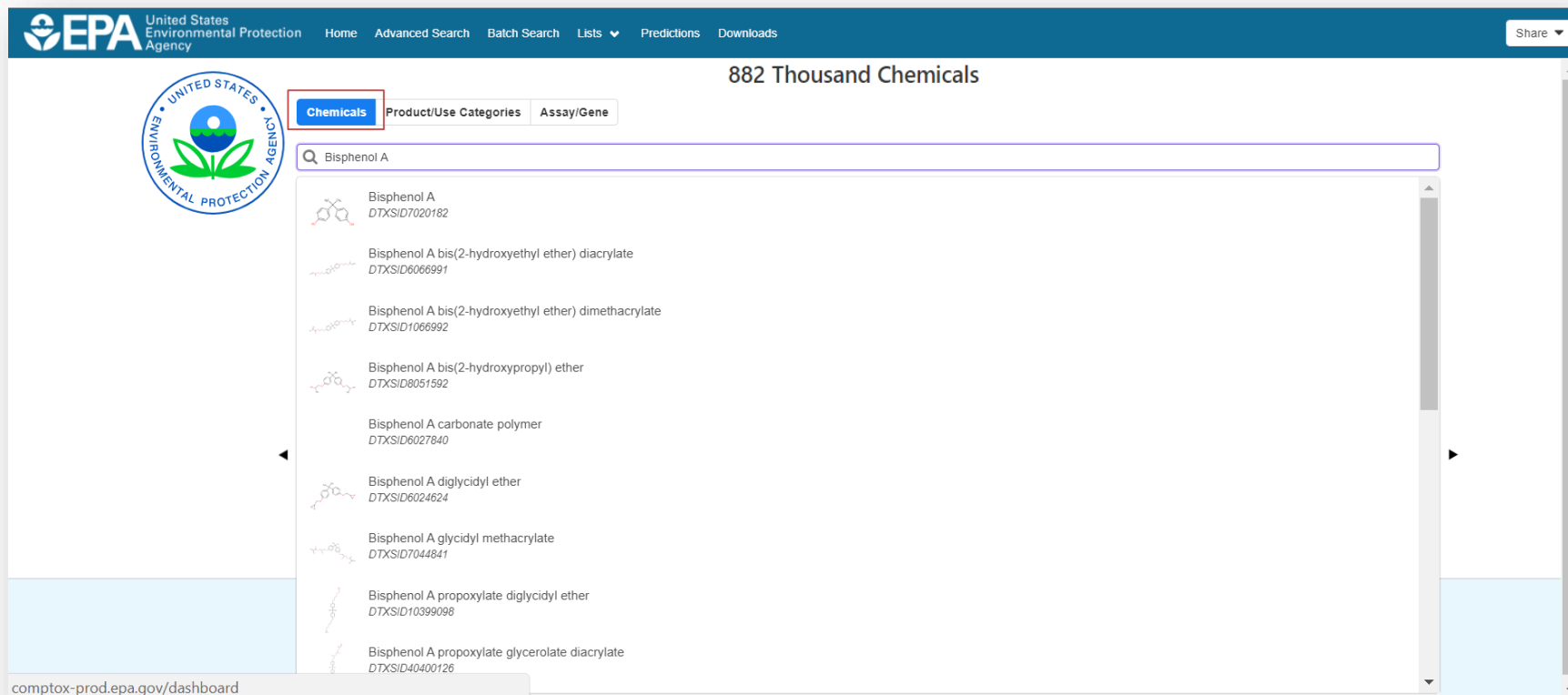
376 of 399 chemicals visible

Chemical Name	DTXSID	Similarity
4-cyclohexylphenol	DTXSID70202556	0.85
4-(1-(4-ethylphenyl)phenyl)phenol	DTXSID70200858	0.85
4-(1-phenylphenyl)phenol	DTXSID70205544	0.85
4,4'-[Thiara (1,1,1-trimethylphenyl)]bis(4-ethylphenol)	DTXSID70203712	0.85
4-(4-ethylphenyl)phenol	DTXSID70208712	0.85

WHAT IS THE DASHBOARD USED FOR?

(and some what's new)

CompTox Dashboard Chemicals



The screenshot displays the EPA CompTox Dashboard interface. At the top, the EPA logo and navigation links (Home, Advanced Search, Batch Search, Lists, Predictions, Downloads) are visible. A search bar contains the text "Bisphenol A". Below the search bar, a list of chemical entries is shown, each with a chemical structure icon, the name of the chemical, and its DTXSID. The "Chemicals" tab is highlighted in the navigation menu. The URL "comptox-prod.epa.gov/dashboard" is visible at the bottom left.

United States Environmental Protection Agency










Home Advanced Search Batch Search Lists Predictions Downloads

Share

882 Thousand Chemicals

Chemicals Product/Use Categories Assay/Gene

Q Bisphenol A

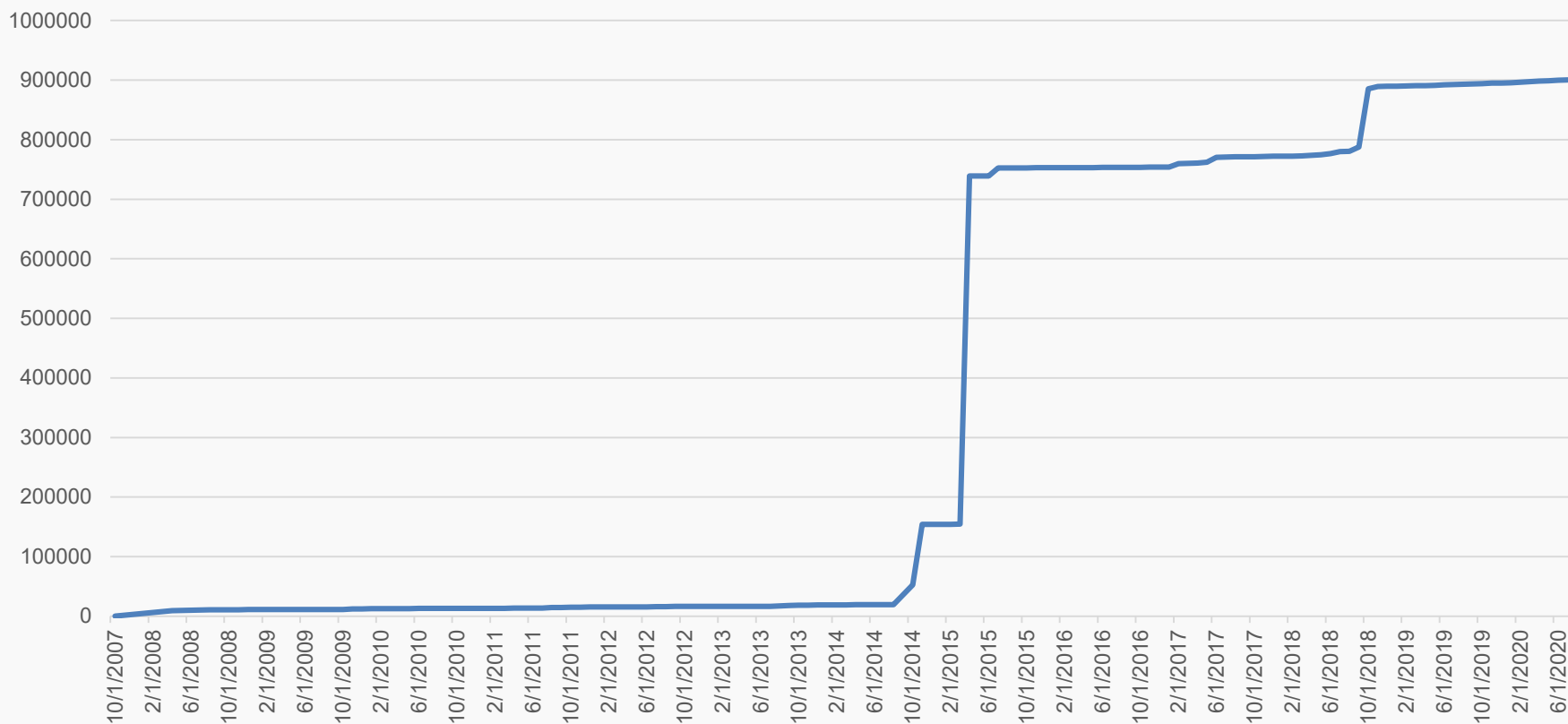
-  Bisphenol A
DTXSID7020182
-  Bisphenol A bis(2-hydroxyethyl ether) diacrylate
DTXSID6066991
-  Bisphenol A bis(2-hydroxyethyl ether) dimethacrylate
DTXSID1066992
-  Bisphenol A bis(2-hydroxypropyl) ether
DTXSID8051592
-  Bisphenol A carbonate polymer
DTXSID6027840
-  Bisphenol A diglycidyl ether
DTXSID6024624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

comptox-prod.epa.gov/dashboard

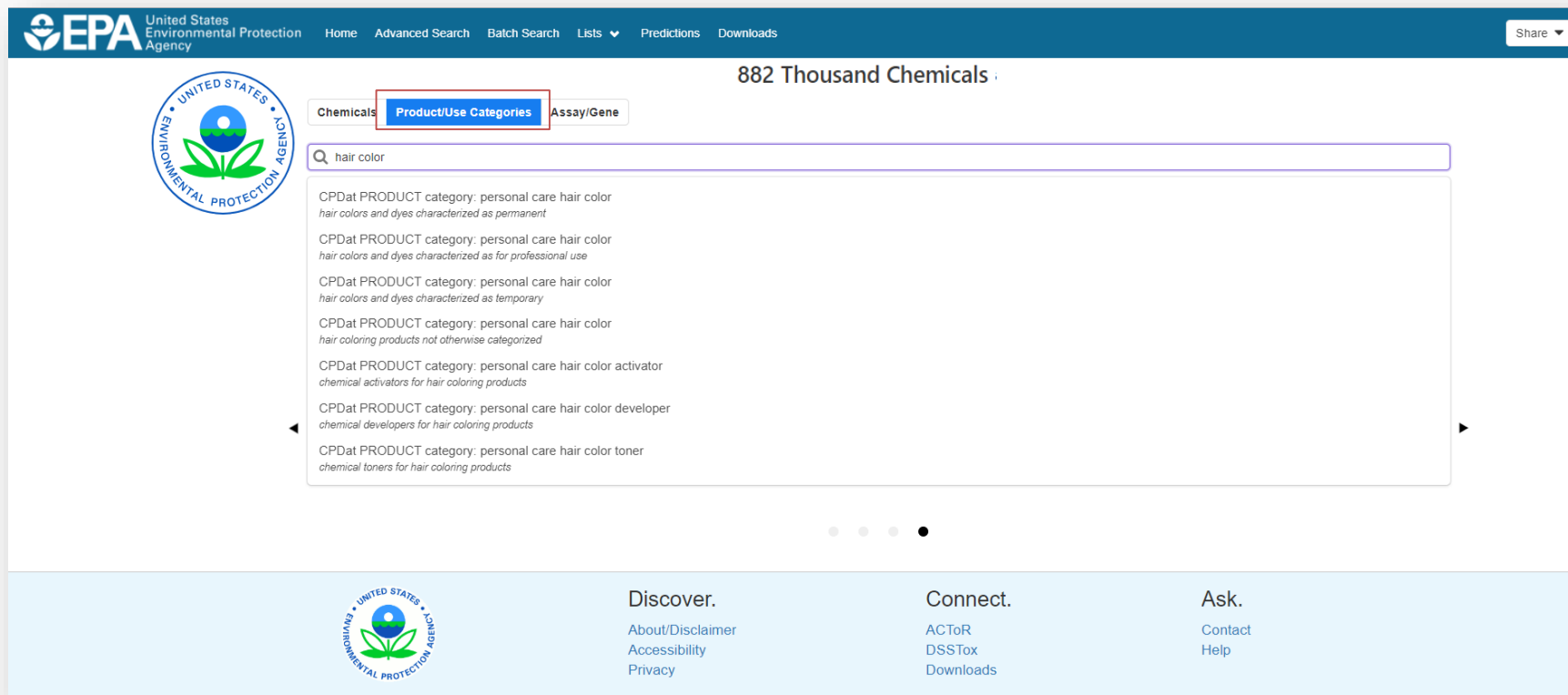
DSSTox growth – 2007 to 2020

>7000 new chemicals added

cumulative (all record)



CompTox Dashboard Products and Use Categories



The screenshot displays the EPA CompTox Dashboard interface. At the top, the EPA logo and navigation menu are visible. The main content area shows a search for "hair color" with results categorized under "Product/Use Categories".

882 Thousand Chemicals

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

Q hair color

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

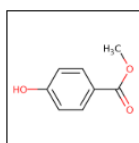
Discover.
[About/Disclaimer](#)
[Accessibility](#)
[Privacy](#)

Connect.
[ACToR](#)
[DSSTox](#)
[Downloads](#)

Ask.
[Contact](#)
[Help](#)

Additional Exposure Data

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

Download 

Columns 

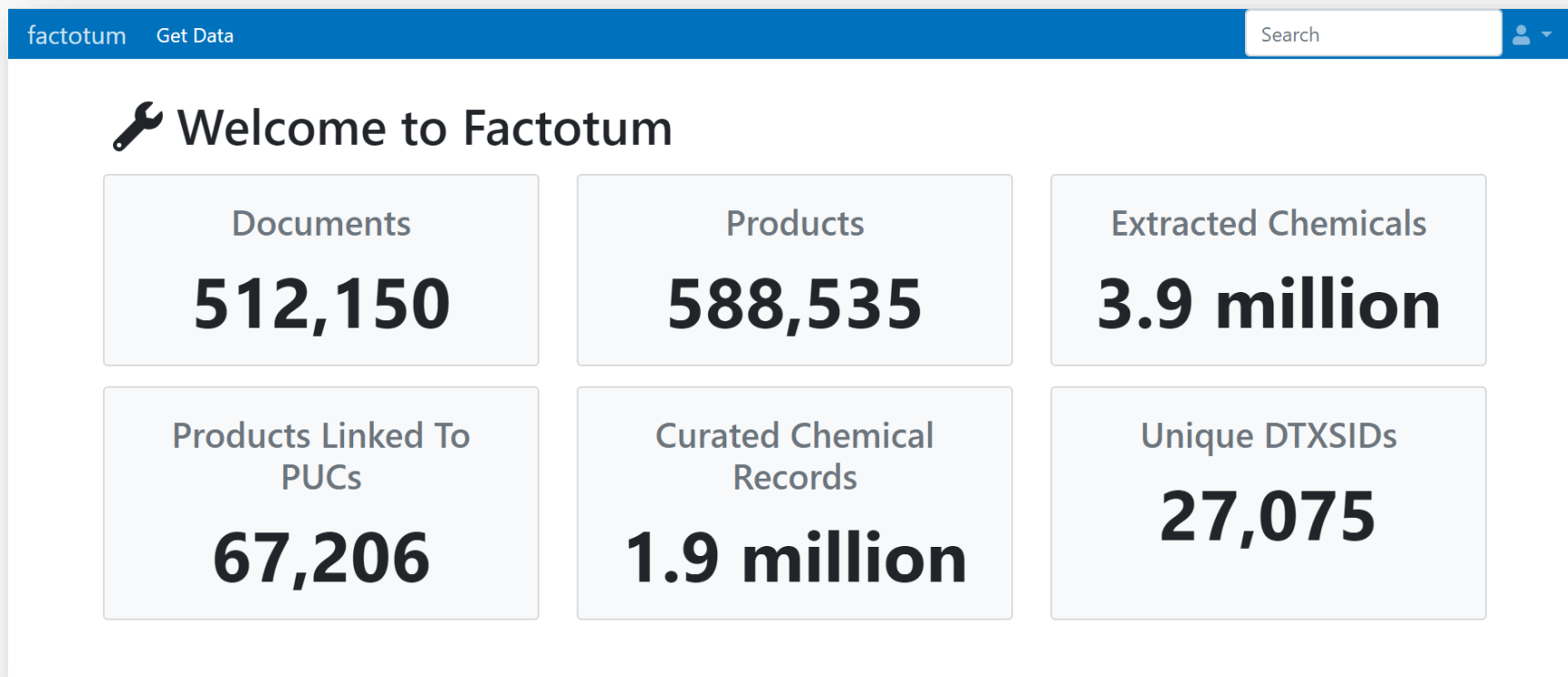
10 

Search query

Product Name 	Minimum Weight Fraction 	Maximum Weight Fraction 	Data Type 	Source 
114 9764 kodak ektachem calibrator kit 5-calibrator 1	0.00	1.00e-2	MSDS	SIRI
114 9764 kodak ektachem calibrator kit 5-calibrator 2	0.00	1.00e-2	MSDS	SIRI
173 6594 ektachem liquid calibrator 16	0.00	1.00e-2	MSDS	SIRI
2540 gabe's grit	0.00	5.00e-3	MSDS	SIRI
276300_ solution_ a e r pads	0.00	1.00e-3	MSDS	SIRI
420 rp super filter coat_ ready-to-use	0.00	1.00e-2	MSDS	SIRI
421 rp super filter coat_ ready-to-use	0.00	1.00e-2	MSDS	SIRI
422 rp super filter coat_ bulk ready-to-use	0.00	1.00e-2	MSDS	SIRI
846 6492 ektachem liquid performance verifier i	0.00	1.00e-2	MSDS	SIRI
846 6492 kodak ektachem liquid performance verifier	0.00	1.00e-2	MSDS	SIRI

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

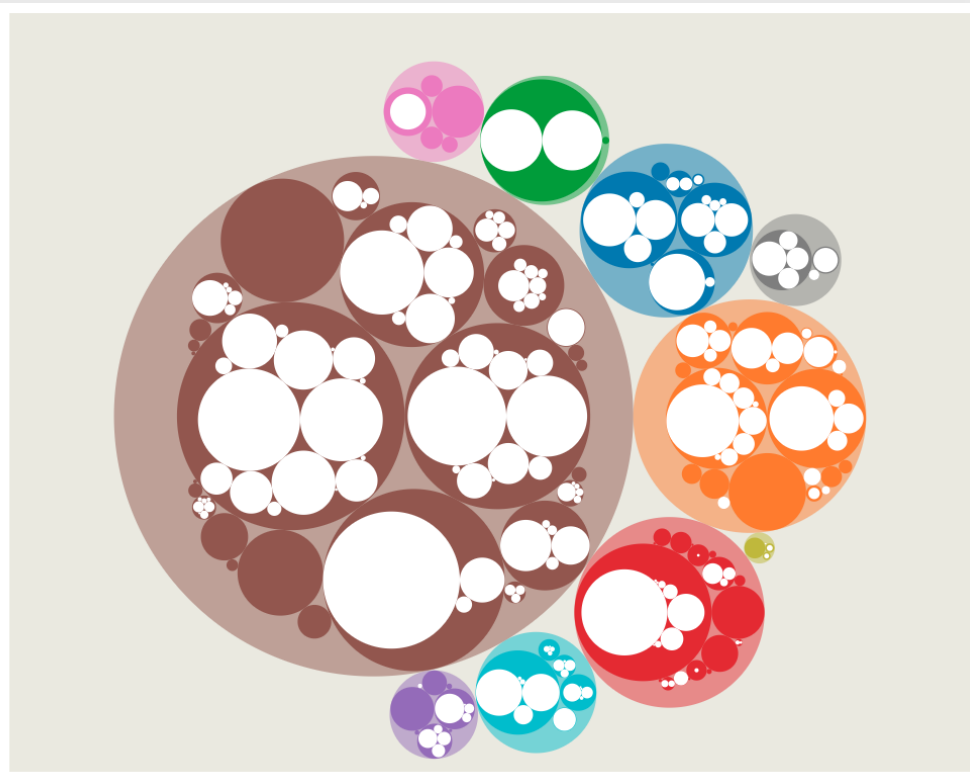
Showing 21 to 30 of 462 records



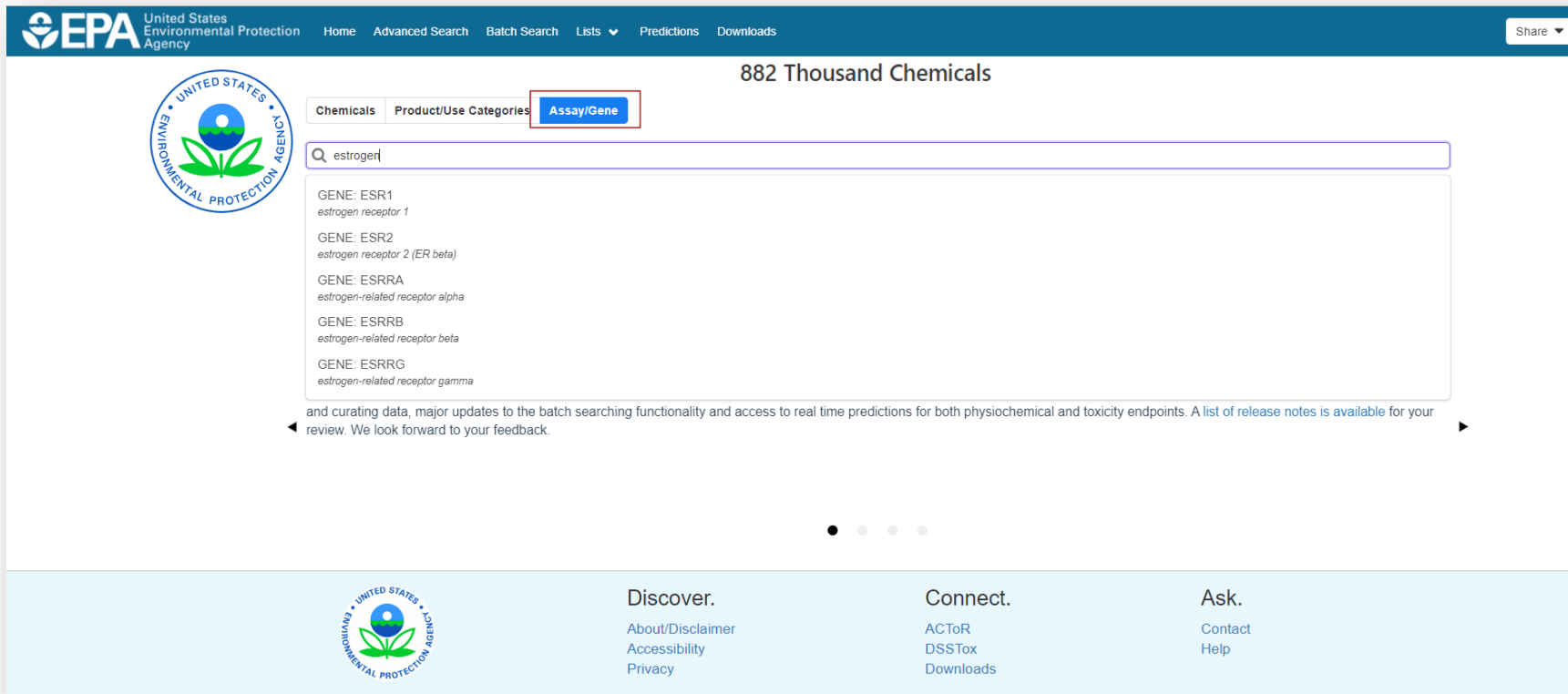
Formulation PUCs

General Category - Product Family - Product Type

> Arts and crafts/Office supplies i	3962
> Cleaning products and household care i	7917
> Electronics/small appliances i	2184
> Home maintenance i	5089
> Landscape/Yard i	1113
> Personal care i	38626
> Pesticides i	1472
> Pet care i	1076
> Sports equipment i	139
> Vehicle i	1743



CompTox Dashboard Assays and Genes



The screenshot displays the EPA CompTox Dashboard interface. At the top, the EPA logo and navigation menu are visible. The main content area shows a search for 'estrogen' with results for various estrogen receptors. The 'Assay/Gene' category is highlighted in the navigation tabs. A search bar contains the text 'estrogen' and a list of search results is displayed below it. The results include:

- GENE: ESR1
estrogen receptor 1
- GENE: ESR2
estrogen receptor 2 (ER beta)
- GENE: ESRA
estrogen-related receptor alpha
- GENE: ESRRB
estrogen-related receptor beta
- GENE: ESRRG
estrogen-related receptor gamma

Below the search results, there is a message: "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."

The footer contains the EPA logo and three columns of links: "Discover." (About/Disclaimer, Accessibility, Privacy), "Connect." (ACToR, DSSTox, Downloads), and "Ask." (Contact, Help).

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

Approx Year	Invitrodb Version (Public)	# assay endpoints	#chemicals (total)	#curve fits (chemical-aid pairs)	#assay endpoints annotated to gene	#unique target genes annotated
2015	2.0	1192	9076	2,244,647	737	377
2018	3.1	1399	9214	3,281,340	1215	442
2019	3.2	1473	9224	3,525,844	1255	443
2020	3.3	1614	9949	3,720,594	1398	492


***SOME
EXAMPLES OF
USAGE***

Find me all "conazoles"

Chemicals
Product/Use Categories
Assay/Gene

🔍

Identifier substring search



[Home](#) [Advanced Search](#) [Batch Search](#) [Lists](#) [Predictions](#) [Downloads](#)

Share

Search Results

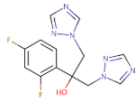
Searched with 'Synonym Substring': Conazole

Select all Download Send to Batch Search Substring

CASRN DTXSID TOXCAST

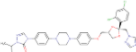
Hide chemicals that are: Filter by Name or CASRN

125 chemicals



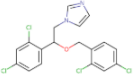
Fluconazole

CASRN:86386-73-4
DTXSID:DTXSID3020627
TOXCAST:11/861



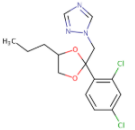
Itraconazole

CASRN:84625-61-6
DTXSID:DTXSID3023180
TOXCAST:43/235



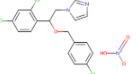
Miconazole

CASRN:60207-90-1
DTXSID:DTXSID6023319
TOXCAST:11/79



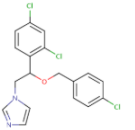
Propiconazole

CASRN:60207-90-1
DTXSID:DTXSID8024280
TOXCAST:259/1045



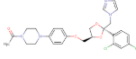
Econazole nitrate

CASRN:24169-02-6
DTXSID:DTXSID6025226
TOXCAST:189/446



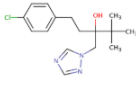
Econazole

CASRN:27220-47-9
DTXSID:DTXSID2029872
TOXCAST:-



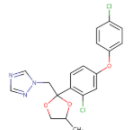
Ketoconazole

CASRN:65277-42-1
DTXSID:DTXSID7029879
TOXCAST:381/913



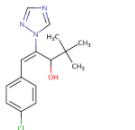
Tebuconazole

CASRN:107534-96-3
DTXSID:DTXSID9032113
TOXCAST:190/947



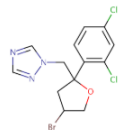
Difenoconazole

CASRN:119446-68-3
DTXSID:DTXSID4032372
TOXCAST:368/1043



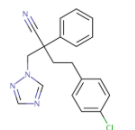
Uniconazole

CASRN:83657-22-1
DTXSID:DTXSID7032505
TOXCAST:-



Bromuconazole

CASRN:116255-48-2
DTXSID:DTXSID9032531
TOXCAST:107/498




Fenbuconazole

CASRN:114369-43-6
DTXSID:DTXSID8032548
TOXCAST:225/1004

What chemicals in what use category?

“What’s in eye liner?”

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share

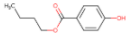
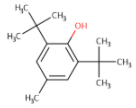
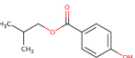
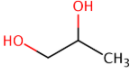
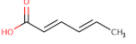
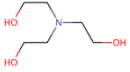


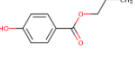
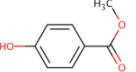
Searched by Product & Use Categories

Results for CPDat Product Category: Make Up And Related: Eye Liner

35 chemicals


Select all Download Send to Batch Search Default CASRN DTXSID TOXCAST

Hide chemicals that are: Filter by Name or CASRN

 <p>Butylparaben CASRN:94-26-8 DTXSID:DTXSID3020209 TOXCAST:117/941</p>	 <p>Butylated hydroxytoluene CASRN:128-37-0 DTXSID:DTXSID2020216 TOXCAST:62/429</p>	 <p>Isobutylparaben CASRN:4247-02-3 DTXSID:DTXSID4020749 TOXCAST:40/235</p>	 <p>1,2-Propylene glycol CASRN:57-55-6 DTXSID:DTXSID0021206 TOXCAST:21/872</p>	 <p>2E,4E-Hexadienoic acid CASRN:110-44-1 DTXSID:DTXSID3021277 TOXCAST:39/865</p>	$O^{2-} Ti^{2+} O^{2-}$ <p>Titanium dioxide CASRN:13463-67-7 DTXSID:DTXSID3021352 TOXCAST:-</p>
 <p>Triethanolamine CASRN:102-71-6 DTXSID:DTXSID9021392 TOXCAST:14/865</p>	 <p>Octadecanoic acid CASRN:57-11-4 DTXSID:DTXSID8021642 TOXCAST:25/862</p>	 <p>cis-Oleyl alcohol CASRN:143-28-2 DTXSID:DTXSID0022010 TOXCAST:0/235</p>	 <p>Propylparaben CASRN:94-13-3 DTXSID:DTXSID4022527 TOXCAST:107/911</p>	 <p>Methylparaben CASRN:99-76-3 DTXSID:DTXSID4022529 TOXCAST:24/886</p>	Cu <p>Copper CASRN:7440-50-8 DTXSID:DTXSID2023985 TOXCAST:-</p>

Access *In Vitro* Bioactivity Data

ToxCast and Tox21



United States
Environmental Protection
Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search all data

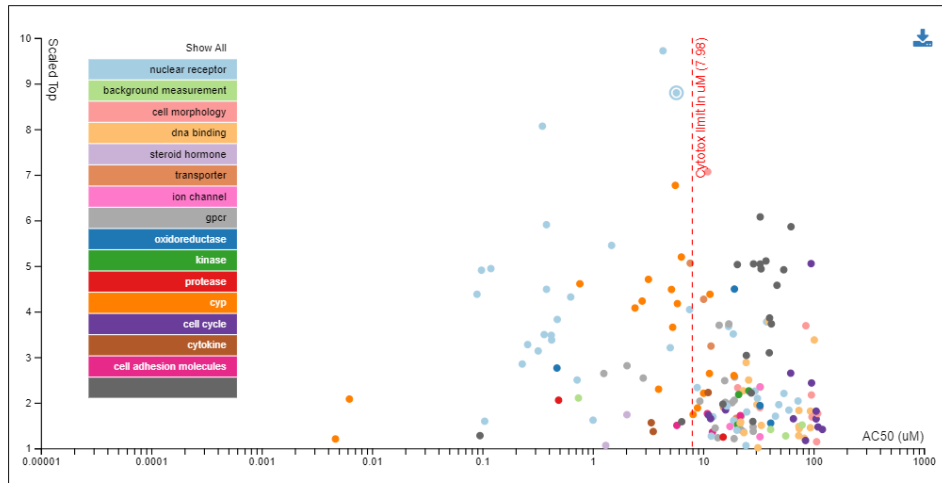
Bisphenol A

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

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY**
 - TOXCAST: SUMMARY**
 - PUBCHEM
 - TOXCAST: DATA
 - TOXCAST: MODELS
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES

Chemical Activity Summary i

TOXCAST DATA



ASSAY DETAILS

AC50 (uM): 5.73
Scaled top: 8.80
Assay Endpoint Name: OT_ER_ERaERa_0480
Assay Description: 742
Gene Symbol: ESR1
Organism: human
Tissue: kidney
Assay Format Type: cell-based
Biological Process Target: protein stabilization
Detection Technology: Protein-fragment Complementation
Analysis Direction: positive
Intended Target Family: nuclear receptor
Description: Data from the assay component OT_ER_ERaERa_0480 was analyzed into 1 assay endpoint. This assay endpoint, OT_ER_ERaERa_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 relatable targets, this assay endpoint is annotated to the 'nuclear receptor' intended target family, where the subfamily is 'steroidal'.

Access *In Vitro* Bioactivity Data ToxCast and Tox21

 **Bisphenol A**
80-05-7 | DTXSID7020182
Searched by Approved Name.

ToxCast/Tox21

QC Data ID	Grade	Description
Tox21_202992	Pass	Purity>90% and MW confirmed
Tox21_400088	Pass	Purity>90% and MW confirmed

Assay Selection 217 Selected

Active Inactive All

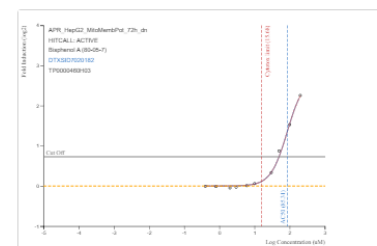
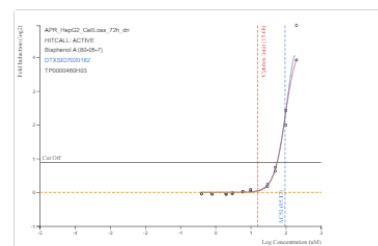
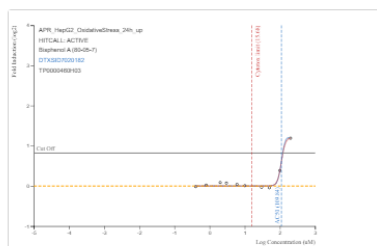
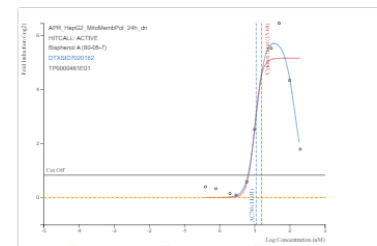
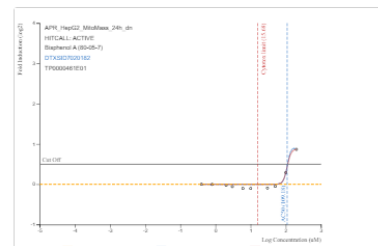
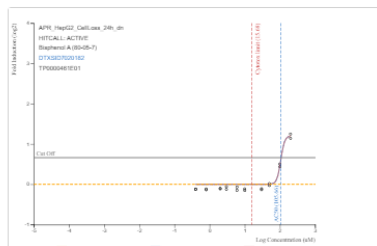
A Single Assay Can Have Multiple Charts

Representative Samples Only

Bioactivity Summary

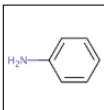
Number of Charts: 217

- Filter assays
- Apredica (8 of 60 selected)
 - Attagene (26 of 165 selected)
 - Bioseek (9 of 174 selected)
 - Novascreen (58 of 167 selected)
 - NHEERL Padilla Lab (1 of 1 selected)
 - CellzDirect (3 of 48 selected)
 - ACEA Biosciences (4 of 6 selected)
 - NHEERL Stoker and Laws Laboratories (2 of 2 selected)
 - Tox21/NCGC (59 of 247 selected)
 - NCCT Simmons Lab (6 of 26 selected)
 - Tanguy Lab (16 of 19 selected)
 - Odyssey Thera (11 of 17 selected)
 - LifeTech/Expression Analysis (5 of 181 selected)
 - Ceetox/OpAns (2 of 24 selected)
 - Stemina Biomarker Discovery (3 of 11 selected)
 - University of Pittsburgh Johnston Lab (4 of 4 selected)



Related Substances

e.g. Transformation Products



Aniline

62-53-3 | DTXSID8020090

Searched by DSSTox Substance Id.

24 of 28 chemicals visible

Select all

Download

Send to Batch Search

Relationship

CASRN

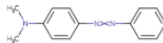
DTXSID

TOXCAST

No Structures

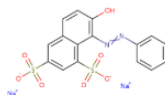
Filter by Name or CASRN

Transformation Parent



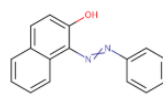
C.I. Solvent Yellow 2
CASRN:60-11-7
DTXSID:DTXSID5020491
TOXCAST:53/235

Transformation Parent



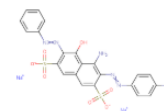
C.I. Acid Orange 10
CASRN:1936-15-8
DTXSID:DTXSID6021082
TOXCAST:35/429

Transformation Parent



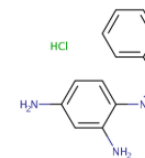
C.I. Solvent Yellow 14
CASRN:842-07-9
DTXSID:DTXSID4021135
TOXCAST:188/923

Transformation Parent



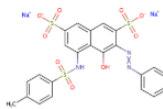
C.I. Acid Black 1, disodium salt
CASRN:1064-48-8
DTXSID:DTXSID1024415
TOXCAST:-

Transformation Parent



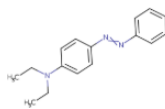
C.I. Basic Orange 2
CASRN:532-82-1
DTXSID:DTXSID0024559
TOXCAST:71/235

Transformation Parent



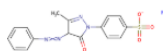
C.I. Acid Red 106, disodium salt
CASRN:6844-74-2
DTXSID:DTXSID1041710
TOXCAST:-

Transformation Parent



C.I. Solvent Yellow 56
CASRN:2481-94-9
DTXSID:DTXSID8041745
TOXCAST:111/481

Transformation Parent



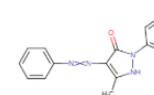
C.I. Acid Yellow 11, sodium salt
CASRN:6359-82-6
DTXSID:DTXSID5047451
TOXCAST:36/433

Transformation Parent



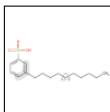
C.I. Solvent Black 3
CASRN:4197-25-5
DTXSID:DTXSID0052091
TOXCAST:-

Transformation Parent



C.I. Solvent Yellow 16
CASRN:4314-14-1
DTXSID:DTXSID5052098
TOXCAST:-

Related Substances for Markush

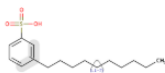
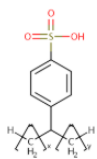
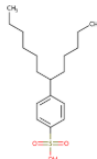
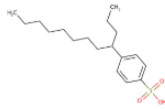
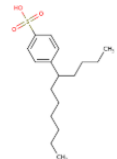
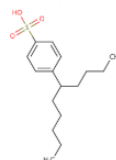
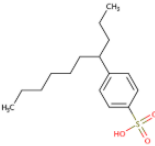
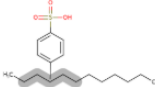
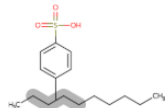



(C10-C16) Alkylbenzenesulfonic acid


68584-22-5 | DTXSID2028723

Searched by DSSTox Substance Id.

Select all Download Send to Batch Search Relationship CASRN DTXSID TOXCAST 20 chemicals Hide chemicals that are: Filter by Name or CASRN

<p>Searched Chemical</p>  <p>(C10-C16) Alkylbenzenesulfonic acid CASRN:68584-22-5 DTXSID:DTXSID2028723 TOXCAST:59/235</p>	<p>Predecessor: Component</p>  <p>Alkylbenzenesulfonate, linear CASRN:42615-29-2 DTXSID:DTXSID3020041 TOXCAST:-</p>	<p>Component</p>  <p>4-(Dodecan-6-yl)benzene-1-sulfonic acid CASRN:23003-92-1 DTXSID:DTXSID30860093 TOXCAST:-</p>	<p>Component</p>  <p>4-(dodecan-4-yl)benzene-1-sulfonic acid CASRN:NOCAS_862870 DTXSID:DTXSID30862870 TOXCAST:-</p>	<p>Component</p>  <p>4-(undecan-5-yl)benzene-1-sulfonic acid CASRN:NOCAS_881097 DTXSID:DTXSID40881097 TOXCAST:-</p>
<p>Component</p>  <p>4-(decan-5-yl)benzene-1-sulfonic acid CASRN:NOCAS_881146 DTXSID:DTXSID70881146 TOXCAST:-</p>	<p>Component</p>  <p>4-(decan-4-yl)benzenesulfonic acid CASRN:NOCAS_891333 DTXSID:DTXSID40891333 TOXCAST:-</p>	<p>Component</p>  <p>C12-linear alkyl benzene sulfonate CASRN:NOCAS_891641 DTXSID:DTXSID90891641 TOXCAST:-</p>	<p>Component</p>  <p>C10-linear alkylbenzenesulfonate CASRN:NOCAS_891689 DTXSID:DTXSID70891689 TOXCAST:-</p>	<p>Markush Child</p>  <p>4-Dodecylbenzenesulfonic acid CASRN:121-65-3 DTXSID:DTXSID8050443 TOXCAST:-</p>

Identifiers to Support Searches


United States Environmental Protection Agency
Home [Advanced Search](#) [Batch Search](#) [Lists](#) [Predictions](#) [Downloads](#)

Copy Share Submit Comment

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

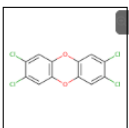
25

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

<u>Synonym</u>	<u>Quality</u>
Bisphenol A	Valid
4,4'-(Propane-2,2-diyl)diphenol	Valid
Phenol, 4,4'-(1-methylethylidene)bis-	Valid
80-05-7 Active CAS-RN	Valid
BPA	Valid
4,4'-Propane-2,2-diylidiphenol	Valid
Phenol, 4,4'-(1-methylethylidene)bis-	Valid
4-06-00-06717 Beilstein Registry Number	Beilstein
(4,4'-Di(4-hydroxyphenyl)dimethylmethane	Good
2,2-Bis(4'-hydroxyphenyl) propane	Good
2,2'-Bis(4-hydroxyphenyl)propane	Good
2,2-BIS-(4-HYDROXY-PHENYL)-PROPANE	Good
2,2-Bis(4-hydroxyphenyl)propane	Good
2,2-Bis(p-hydroxyphenyl)propane	Good
2,2-Di(4-Hydroxyphenyl) Propane	Good

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

1495 of 1495 articles loaded...

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

Download / Send to...

<input type="checkbox"/>	dioxin	cancer	mortality ↓	Total	PMID	Year	Title	Authors	Journal
<input type="checkbox"/>	6	6	9	21	8734824	1996	Cancer mortality in German male workers exposed to p...	Becher; Flesch-Janys; Kauppinen; Kogevinas; Stei...	Cancer causes & control : CCC
<input type="checkbox"/>	3	9	9	21	1985242	1991	Cancer mortality in workers exposed to 2,3,7,8-tetrachlo...	Fingerhut; Halperin; Marlow; Piacitelli; Honchar; Sw...	The New England journal of medicine
<input type="checkbox"/>	3	9	8	20	27897234	2016	Association between dioxin and cancer incidence and m...	Xu; Ye; Huang; Chen; Wu; Huang; Hu; Xia; Wu	Scientific reports
<input type="checkbox"/>	3	5	8	16	9599713	1998	Estimation of the cumulated exposure to polychlorinated...	Flesch-Janys; Steindorf; Gurn; Becher	Environmental health perspectives
<input type="checkbox"/>	9	7	8	24	9199536	1997	Cancer mortality in workers exposed to phenoxy herbici...	Kogevinas; Becher; Benn; Bertazzi; Boffetta; Bueno...	American journal of epidemiology
<input type="checkbox"/>	6	5	8	19	7485063	1995	Exposure to polychlorinated dioxins and furans (PCDD/...	Flesch-Janys; Berger; Gurn; Manz; Nagel; Waltsgot...	American journal of epidemiology
<input type="checkbox"/>	3	5	8	16	1681339	1991	Cancer mortality among workers in chemical plant conta...	Manz; Berger; Dwyer; Flesch-Janys; Nagel; Waltsgott	Lancet (London, England)
<input type="checkbox"/>	1	2	7	10	19297337	2009	Mortality in employees at a New Zealand agrochemical ...	McBride; Burns; Herbison; Humphry; Bodner; Collins	Occupational medicine (Oxford, England)
<input type="checkbox"/>	1	2	7	10	2139014	1990	Thirty-four-year mortality follow-up of BASF employees ...	Zober; Messerer; Huber	International archives of occupational and environm...
<input type="checkbox"/>	1	4	6	11	2729256	1989	Ten-year mortality study of the population involved in th...	Bertazzi; Zocchetti; Pesatori; Guercilena; Sanarico; ...	American journal of epidemiology
<input type="checkbox"/>	7	0	5	12	27932487	2016	Mortality risk among workers with exposure to dioxins.	Collins; Bodner; Aylward; Bender; Anteau; Wilken; ...	Occupational medicine (Oxford, England)
<input type="checkbox"/>	2	5	5	12	21810927	2011	Plasma dioxin levels and cause-specific mortality in an ...	Boers; Portengen; Turner; Bueno-de-Mesquita; Hee...	Occupational and environmental medicine

Mass and Formula Searches Supporting Mass Spectrometry


Advanced Search

Mass Search



Min/Max

Adduct
 All Adducts Choose adduct from dropdown

Mass Error ppm




Molecular Formula Search

MS Ready Formula  Exact Formula 

Formula

Please use the format of the following example: C6H8O2 or C6H(8-10)O(0-2)



Generate Molecular Formula(e)

Min/Max


Adduct

Mass Error ppm

https://epa.gov

Advanced Searches

Mass Based Search

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share

Search Results

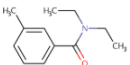
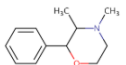
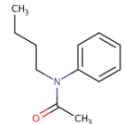
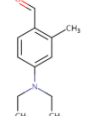
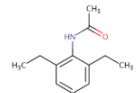
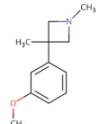
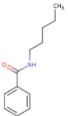
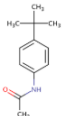
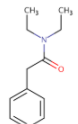
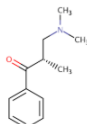
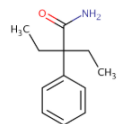
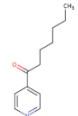
Searched by Mass: 191.131 +/- 5.0 ppm.

335 of 335 chemicals visible

Select all Download Send to Batch Search Mass Difference

DTXSID CASRN TOXCAST Mass Diff

Multicomponent Chemicals Filter by Name or CASRN

 <p>DEET DTXSID:DTXSID2021995 CASRN:134-62-3 TOXCAST:29/929 Mass Diff:0.000014</p>	 <p>Phendimetrazine DTXSID:DTXSID1023447 CASRN:634-03-7 TOXCAST:- Mass Diff:0.000014</p>	 <p>N-Butylacetanilide DTXSID:DTXSID2042197 CASRN:91-49-6 TOXCAST:- Mass Diff:0.000014</p>	 <p>Benzaldehyde, 4-(diethylamino)-2-methyl- DTXSID:DTXSID4059041 CASRN:92-14-8 TOXCAST:- Mass Diff:0.000014</p>	 <p>Acetanilide, 2',6'-diethyl- DTXSID:DTXSID90168148 CASRN:16665-89-7 TOXCAST:- Mass Diff:0.000014</p>	 <p>Azetidine, 1,3-dimethyl-3-(m-methoxyphenyl)- DTXSID:DTXSID40173560 CASRN:19832-26-9 TOXCAST:- Mass Diff:0.000014</p>
 <p>Benzamide, N-pentyl- DTXSID:DTXSID20174196 CASRN:20308-43-4 TOXCAST:- Mass Diff:0.000014</p>	 <p>p-t-Butylacetanilide DTXSID:DTXSID80174238 CASRN:20330-45-4 TOXCAST:- Mass Diff:0.000014</p>	 <p>N,N-Diethylphenylacetamide DTXSID:DTXSID00179048 CASRN:2431-96-1 TOXCAST:- Mass Diff:0.000014</p>	 <p>3-(Dimethylamino)-2-methylpropiofenone DTXSID:DTXSID60180796 CASRN:26171-90-6 TOXCAST:- Mass Diff:0.000014</p>	 <p>Butyramide, 2-ethyl-2-phenyl- DTXSID:DTXSID60184653 CASRN:30568-39-9 TOXCAST:- Mass Diff:0.000014</p>	 <p>1-Heptanone, 1-(4-pyridyl)- DTXSID:DTXSID40186594 CASRN:32941-30-3 TOXCAST:- Mass Diff:0.000014</p>

Journal of Cheminformatics

[Home](#) [About](#) [Articles](#) [Submission Guidelines](#)

[Abstract](#)

[Background](#)

[Methods](#)

[Results and discussion](#)

[Conclusions](#)

[Declarations](#)

[References](#)

Methodology | [Open Access](#)

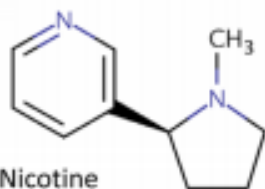
"MS-Ready" structures for non-targeted high-resolution mass spectrometry screening studies

[Andrew D. McEachran](#) , [Kamel Mansouri](#), [Chris Grulke](#), [Emma L. Schymanski](#), [Christoph Ruttkies](#) and [Antony J. Williams](#) 

Journal of Cheminformatics 2018 **10**:45

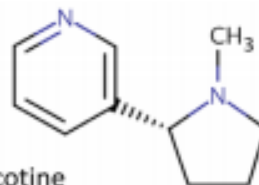
<https://doi.org/10.1186/s13321-018-0299-2> | © The Author(s) 2018

Received: 16 May 2018 | **Accepted:** 21 August 2018 | **Published:** 30 August 2018



Nicotine

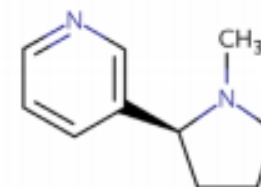
CN1CCC[C@H]1C1=CN=CC=C1
 DTXSID1020930 | SNICXCGAKADSCV
 54-11-5 | **162.1157** | 0.929 | **72**
 Tox: **yes** | Expo: **yes** | Bioassay: **yes**



D-Nicotine

CN1CCC[C@@H]1C1=CN=CC=C1
 DTXSID004635 | SNICXCGAKADSCV
 25162-00-9 | **162.1157** | 0.929 | **20**
 Tox: **no** | Expo: **yes** | Bioassay: **yes**

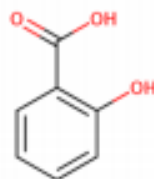
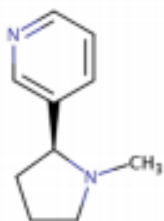
LEGEND: Name, SMILES
 DTXSID | InChIKey 1st Block
 CAS | Monoiso. Mass | logP | Sources
 Data on: Toxicity | Exposure | Bioassays



HCl

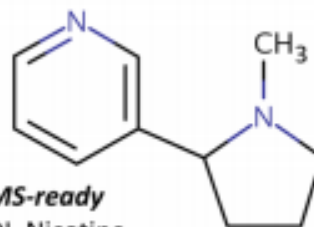
Nicotine hydrochloride

Cl.CN1CCC[C@H]1C1=CN=CC=C1
 DTXSID602093 | HDJBTCAJIMNXEW
 2820-51-1 | **198.0924** | 0.929 | **9**
 Tox: **no** | Expo: **yes** | Bioassay: **yes**



Benzoic acid, 2-hydroxy-, compd. with
 3-[(2S)-1-methyl-2-pyrrolidinyl]pyridine (1:1)

OC(=O)C1=C(O)C=CC=C1.CN1CCC[C@H]1C1=CN=CC=C1
 DTXSID5075319 | AIBWPBUAKCMKNS
 29790-52-1 | **300.1474** | 0.929 | **6**
 Tox: **no** | Expo: **yes** | Bioassay: **no**

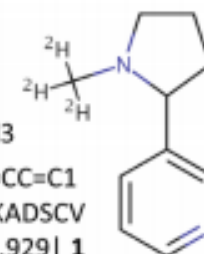


MS-ready
 DL-Nicotine

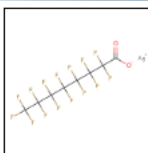
CN1CCCC1C1=CN=CC=C1
 DTXSID3048154 | SNICXCGAKADSCV
 22083-74-5 | **162.1157** | 0.953 | **9**
 Tox: **yes** | Expo: **no** | Bioassay: **yes**

DL-Nicotine-d3

[2H]C([2H])([2H])N1CCCC1C1=CN=CC=C1
 DTXSID80442666 | SNICXCGAKADSCV
 69980-24-1 | **165.1345** | 0.929 | **1**
 Tox: **no** | Expo: **no** | Bioassay: **no**



Find me all salts of...



Silver perfluorooctanoate

335-93-3 | DTXSID00880127

Searched by DSSTox Substance Id.

Quality Control Notes

MS-Ready Mappings of Perfluorooctanoic acid (Isotopes pre-filtered)

16 of 22 chemicals visible

Select all

Download

Send to Batch Search

Default

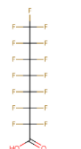
CASRN

DTXSID

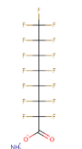
TOXCAST

Isotopes

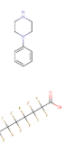
Filter by Name or CASRN



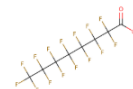
Perfluorooctanoic acid
CASRN:335-67-1
DTXSID:DTXSID8031865
TOXCAST:80/1012



Ammonium perfluorooctanoate
CASRN:3825-26-1
DTXSID:DTXSID8037708
TOXCAST:58/798



pentadecafluorooctanoic acid- 1-phenyl...
CASRN:1514-68-7
DTXSID:DTXSID60293633
TOXCAST:-



Pentadecafluorooctanoic acid--pyridine ...
CASRN:95658-47-2
DTXSID:DTXSID70562266
TOXCAST:-



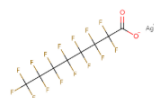
Pentadecafluorooctanoic acid--piperazin...
CASRN:423-52-9
DTXSID:DTXSID50712909
TOXCAST:-



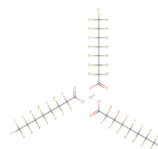
Sodium perfluorooctanoate
CASRN:335-95-5
DTXSID:DTXSID40880025
TOXCAST:-



Potassium perfluorooctanoate
CASRN:2395-00-8
DTXSID:DTXSID00880026
TOXCAST:-



Silver perfluorooctanoate
CASRN:335-93-3
DTXSID:DTXSID00880127
TOXCAST:-



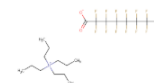
Chromium(3+) perfluorooctanoate
CASRN:68141-02-6
DTXSID:DTXSID00880581
TOXCAST:-



Perfluorooctanoate N,N,N-trimethylmet...
CASRN:32609-65-7
DTXSID:DTXSID20881358
TOXCAST:-



Perfluorooctanoate ion(1-)
CASRN:45285-51-6
DTXSID:DTXSID40892486
TOXCAST:-

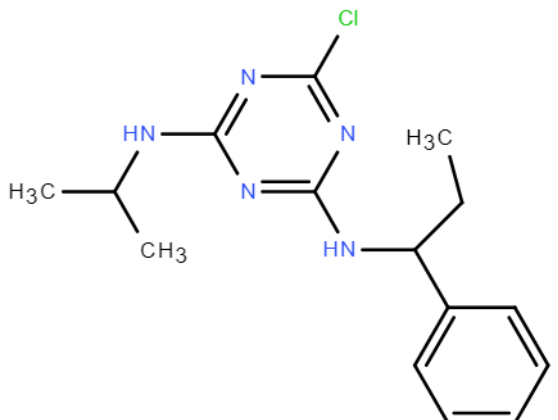


Tetrapropylammonium perfluorooctano...
CASRN:277749-00-5
DTXSID:DTXSID00893530
TOXCAST:-

Real-Time Predictions

Predictions

Q Atrazine



130%

Select properties to predict

H T.E.S.T.

C

N

O

S

P

F

Cl

Br

I

PT

- Toxicological properties
 - 96 hour fathead minnow LC50
 - 48 hour D. magna LC50
 - 48 hour T. pyriformis IGC50
 - 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

Chiral

Real-Time Predictions

Provider: T.E.S.T.

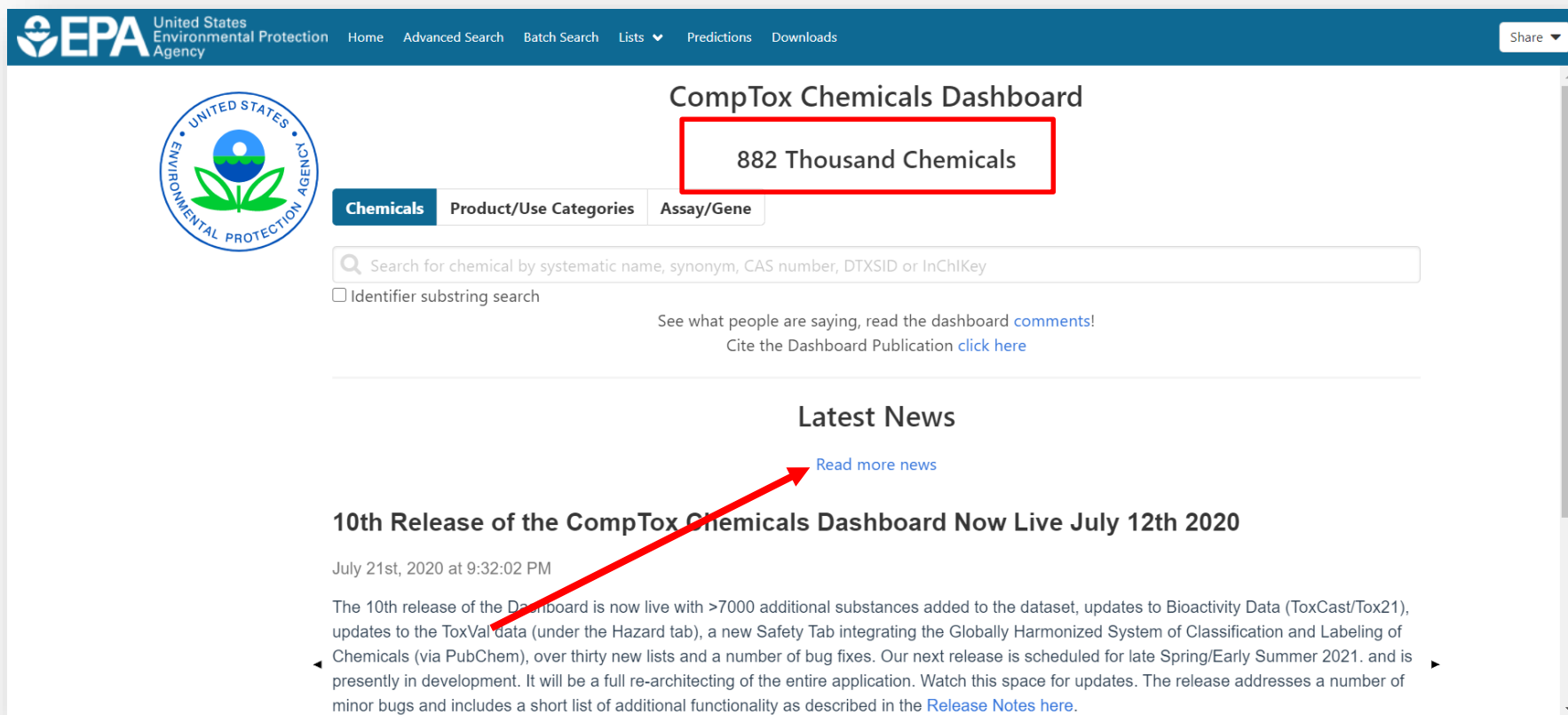
[Download Summary](#)

Property	Experimental Value	Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50		5.000 -Log10(mol/L) 3.057 mg/L	5.194 -Log10(mol/L) 1.958 mg/L	5.592 -Log10(mol/L) 0.783 mg/L	5.151 -Log10(mol/L) 2.158 mg/L	4.064 -Log10(mol/L) 26.414 mg/L
48 hour D. magna LC50		4.827 -Log10(mol/L) 4.553 mg/L	4.920 -Log10(mol/L) 3.679 mg/L	5.266 -Log10(mol/L) 1.657 mg/L	5.317 -Log10(mol/L) 1.473 mg/L	3.806 -Log10(mol/L) 47.846 mg/L
48 hour T. pyriformis IGC50		5.209 -Log10(mol/L) 1.892 mg/L	5.074 -Log10(mol/L) 2.581 mg/L			5.343 -Log10(mol/L) 1.387 mg/L
Oral rat LD50		2.059 -Log10(mol/kg) 2669.702 mg/kg	2.028 -Log10(mol/kg) 2869.132 mg/kg			2.090 -Log10(mol/kg) 2484.135 mg/kg
Bioconcentration factor		1.285 Log10 19.279	1.328 Log10 21.270	1.592 Log10 39.048	1.716 Log10 51.953	0.505 Log10 3.201
Developmental toxicity		true	true	true		
Ames mutagenicity		false	false			false
Estrogen Receptor RBA						
Estrogen Receptor Binding		false	false	false	false	
Normal boiling point		372.1 °C	331.0 °C		479.8 °C	305.5 °C
Melting point		133.9 °C	126.4 °C		138.6 °C	136.7 °C
Flash point		232.7 °C	282.4 °C		240.2 °C	175.7 °C

***NEW
CAPABILITIES,
DATA AND LISTS***

Watch for our news

https://comptox.epa.gov/dashboard/news_info



The screenshot shows the EPA CompTox Chemicals Dashboard. At the top left is the EPA logo and navigation links: Home, Advanced Search, Batch Search, Lists, Predictions, and Downloads. A 'Share' button is in the top right. The main heading is 'CompTox Chemicals Dashboard' with a red box around the text '882 Thousand Chemicals'. Below this are three tabs: 'Chemicals' (selected), 'Product/Use Categories', and 'Assay/Gene'. A search bar is present with the text 'Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey'. Below the search bar is a checkbox for 'Identifier substring search' and links for 'See what people are saying, read the dashboard comments!' and 'Cite the Dashboard Publication click here'. The 'Latest News' section features a red arrow pointing to the 'Read more news' link. The news item is titled '10th Release of the CompTox Chemicals Dashboard Now Live July 12th 2020' and dated 'July 21st, 2020 at 9:32:02 PM'. The text of the news item describes the 10th release, mentioning the addition of >7000 substances, updates to Bioactivity Data (ToxCast/Tox21), ToxVal data, and a new Safety Tab. It also mentions that the next release is scheduled for late Spring/Early Summer 2021 and includes a full re-architecting of the application. A red arrow points from the 'Read more news' link to the news item.

United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share

CompTox Chemicals Dashboard

882 Thousand Chemicals

Chemicals Product/Use Categories Assay/Gene

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey

Identifier substring search

See what people are saying, read the dashboard [comments!](#)
Cite the Dashboard Publication [click here](#)

Latest News

[Read more news](#)

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

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

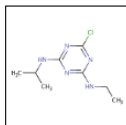
The 10th release of the Dashboard is now live with >7000 additional substances added to the dataset, updates to Bioactivity Data (ToxCast/Tox21), updates to the ToxVal data (under the Hazard tab), a new Safety Tab integrating the Globally Harmonized System of Classification and Labeling of Chemicals (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

New Safety Tab Integrating PubChem GHS Data



Atrazine

1912-24-9 | DTXSID9020112

Searched by DSSTox Substance Id.

GHS Data

Print Page


[PUBCHEM](#) > [ATRAZINE](#) > [LABORATORY CHEMICAL SAFETY SUMMARY \(LCSS\)](#) > [GHS CLASSIFICATION](#)

CID 2256

Atrazine

GHS Classification

Showing 6 of 6

Pictogram(s)	 Irritant 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	P260, P261, P272, P273, P280, P302+P352, P314, P321, P333+P313, P363, P391, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

SAFETY

GHS DATA

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

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

Download Columns 10 Search query Copy page URL

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
CECSCREEN	NORMAN: HBM4EU CECscreen: Screening List for Chemicals of Emerging Concern	2020-07-22	56377	HBM4EU CECscreen is a suspect screening list for Chemicals of Emerging Concern (CECs) plus metadata and predicted Phase 1 metabolites
ROSINS	List of chemicals related to Rosins	2020-07-21	872	Rosin is a solid form of resin obtained from pines and some other plants, mostly conifers.
PFASDEV1	PFAS/EPA PFAS chemicals without explicit structures	2020-07-16	1072	List of PFAS chemicals without explicit structures - polymers and other UVCB chemicals
AROMATICAMINES	REACH: Appendix 8 lists aromatic amines associated with azocolourants	2020-07-12	22	REACH Appendix 8: aromatic amines associated with azocolourants.
CPDAT	EPA: CPDAT, Chemical and Products Database	2020-07-09	37143	Chemicals contained in the EPA's Chemical and Products Database
EPCRALISTS	Consolidated List of Lists under EPCRA/CERCLA/CAA §112(r) (June 2019 Version)	2020-07-07	1363	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).

Disinfectant By-Products

82 to 619 chemicals

LIST: Disinfection By-products (Richardson et al)

 Identifier substring search

List Details

Description: A list of disinfection by-products associated with RICHARDSON, S. D. Disinfection By-Products: Formation and Occurrence in Drinking Water. Chapter 2, J.O. Nriagu (ed.), Encyclopedia of Environmental Health. Elsevier Science Inc., Burlington, MA, 2:110-136, (2011).

Number of Chemicals: 619

619 chemicals

Select all

Download

Send to Batch Search

Default

↑

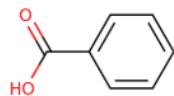
CASRN x

DTXSID x

TOXCAST x

Hide chemicals that are:

Filter by Name or CASRN

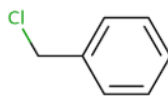


Benzoic acid

CASRN:65-85-0

DTXSID:DTXSID6020143

TOXCAST:13/857

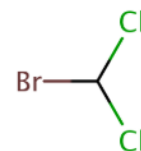


Benzyl chloride

CASRN:100-44-7

DTXSID:DTXSID0020153

TOXCAST:3/235



Bromodichloromethane

CASRN:75-27-4

DTXSID:DTXSID1020198

TOXCAST:0/235



2-Bromo-1-ethanol

CASRN:540-51-2

DTXSID:DTXSID8020200

TOXCAST:5/235

Consolidated List of Lists under EPCRA/CERCLA/CAA §112(r) (June 2019 Version)

Search EPCRALISTS Chemicals

Identifier substring search

List Details

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

Select all

Download

Send to Batch Search

Default

↑

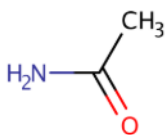
CASRN x

DTXSID x

TOXCAST x

Hide chemicals that are:

Filter by Name or CASRN

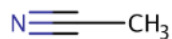


Acetamide

CASRN:60-35-5

DTXSID:DTXSID7020005

TOXCAST:17/864

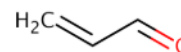


Acetonitrile

CASRN:75-05-8

DTXSID:DTXSID7020009

TOXCAST:0/235

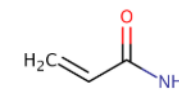


Acrolein

CASRN:107-02-8

DTXSID:DTXSID5020023

TOXCAST:2/235



Acrylamide

CASRN:79-06-1

DTXSID:DTXSID5020027

TOXCAST:22/887

Curated Wikipedia >12,000 chemicals

LIST: Wikipedia chemicals

 Identifier substring search

List Details

Description: Wikipedia includes data for thousands of chemicals. ChemBoxes and DrugBoxes includes data such as CAS Registry Numbers, SMILES and InChIs. This list is an assembly from various Wikipedia pages and is a list under ongoing curation and expansion.

Number of Chemicals: 12861

1250 of 12861 chemicals loaded

Select all

Download

Send to Batch Search

Default



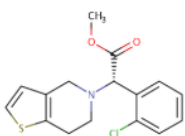
CASRN x

DTXSID x

TOXCAST x

Hide chemicals that are:

Filter by Name or CASRN

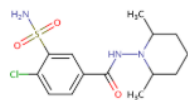


Clopidogrel

CASRN:113665-84-2

DTXSID:DTXSID6022848

TOXCAST:-

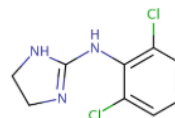


Clopamide

CASRN:636-54-4

DTXSID:DTXSID1022847

TOXCAST:0/79

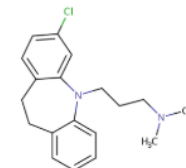


Clonidine

CASRN:4205-90-7

DTXSID:DTXSID6022846

TOXCAST:0/235



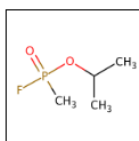
Clomipramine

CASRN:303-49-1

DTXSID:DTXSID6022844

TOXCAST:82/235

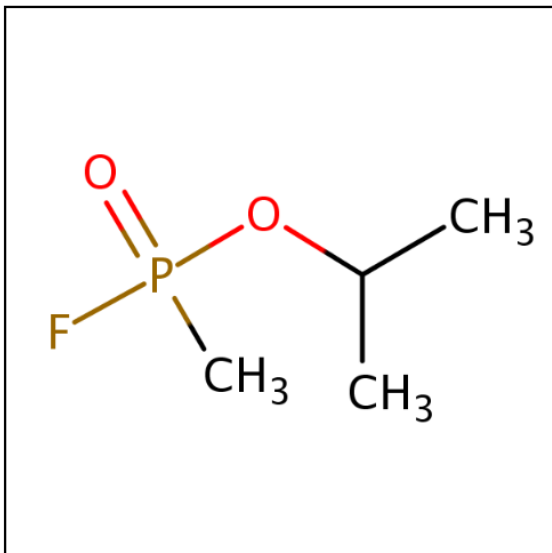
Wikipedia serves the “snippet”



Sarin

107-44-8 | DTXSID0042371

Searched by DSSTox Substance Id.



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  Mol File  Find All Chemicals

 **Average Mass:** 140.094 g/mol  Isotope Mass Distribution

 **Monoisotopic Mass:** 140.040245 g/mol

- 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



[Metabolites](#). 2020 Jun; 10(6): 260.

PMCID: PMC7345619

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

PMID: [32585902](https://pubmed.ncbi.nlm.nih.gov/32585902/)

Revisiting Five Years of CASMI Contests with EPA Identification Tools

[Andrew D. McEachran](#),^{1,*} [Alex Chao](#),¹ [Hussein Al-Ghoul](#),¹ [Charles Lowe](#),² [Christopher Grulke](#),² [Jon R. Sobus](#),²
and [Antony J. Williams](#)^{2,*}

Lists provide a landscape overview

Presence in Lists

Federal

- TOXCASST_PhaseII - EPA ToxCast Screening Library (Phase II Subset)
- TOXCASST_PhaseIII - EPA ToxCast Screening Library (Phase II Subset)
- TOXCASST_ph2 - EPA ToxCast Screening Library (ph2 Subset)
- CHEMINV: EPA Chemical Inventory for ToxCast
- TOXCASST: 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
- TOXCASST: 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
- EPA|LIST: Article "Workflow for Defining Reference Chemicals for Assessing Performance of In Vitro Assays"
- NORMAN: REACH Chemicals List Provided to NORMAN Network
- NORMAN: Norman Network Suspect Screening List (SUSDAT)
- EPA: CPDAT, Chemical and Products Database
- Global harmonization system aggregated chemical data list (skin and eyes)
- MASSPECDB: Thermo's mzCloud Database
- NORMAN: Combined 2000/2006 EU Cosmetic Ingredients Inventory
- WATER: STOFF-IDENT Database of Water-Relevant 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)
- EPA: Toxicity Values Version 5 (Aug 2018)
- LIST: Wikipedia chemicals
- LIST: Hazardous Substances Data Bank
- PESTICIDES|EPA: List of Inert Ingredients Food and Nonfood Use UPDATED 10/25/2019

- Batch search a list of chemicals to identify presence in >280 lists

LIST: Azo Dyes

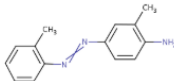
Search AZODYES Chemicals
 Identifier substring search

List Details

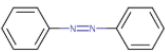
Description: List of Azo Dyes assembled from public sources including Wikipedia
Number of Chemicals: 274

271 chemicals

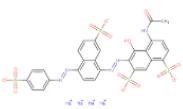
Select all Download Send to Batch Search Default CASRN DTXSID TOXCAST Hide chemicals that are: Filter by Name or CASRN



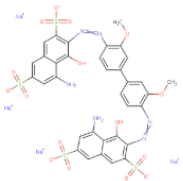
o-Aminoazotoluene
CASRN:97-56-3
DTXSID:DTXSID1020069
TOXCAST:336/929



Azobenzene
CASRN:103-33-3
DTXSID:DTXSID8020123
TOXCAST:33/874



Black PN
CASRN:2519-30-4
DTXSID:DTXSID2020183
TOXCAST:-



C.I. Direct Blue 15
CASRN:2429-74-5
DTXSID:DTXSID7020186
TOXCAST:-

Select lists of Interest & Export File










Batch Search



Step Four: Select Data Output Format and Choose Data Fields to Download

Please enter one identifier per line ✕

Select Input Type(s)

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

Enter Identifiers to Search (One per line. Searches should be limited to <5000 identifiers.)

DTXSID1020069
DTXSID8020123
DTXSID2020183
DTXSID7020186
DTXSID3020201
DTXSID9020324
DTXSID5020491
DTXSID6020511
DTXSID6021082
DTXSID1021118

Select Output Format:



📄 Excel ▼

⬇️ Download

Customize Results

- Select All
- Select All in Lists

Chemical Identifiers

- DTXSID 
- Chemical Name 

Presence in Lists:

- 40CFR116.4 Designation of Hazardous Substances (Above Ground Storage Tanks) [🔗](#)
- 40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities [🔗](#)
- AEGLS: Acute Exposure Guideline Levels [🔗](#)
- ANDROGEN: Androgen Receptor Chemicals [🔗](#)

Cross-walking lists of interest

	A	B	C	D	E	F	G	H	I
	DTXSID	PREFERRED_NAME	CANADADSL	OEHHA	EPCRALISTS	ECOTOX_V2	EDSPUOC	CPDAT	TRIRELEASE
1	DTXSID1020069	o-Aminoazotoluene	Y	Y	Y	Y	Y	Y	Y
2	DTXSID8020123	Azobenzene	Y	Y	-	Y	Y	Y	-
3	DTXSID2020183	Black PN	-	-	-	-	-	Y	-
4	DTXSID7020186	C.I. Direct Blue 15	Y	Y	-	-	Y	Y	-
5	DTXSID3020201	C.I. Direct Brown 95	Y	Y	Y	Y	Y	Y	Y
6	DTXSID9020324	Chocolate Brown HT	-	-	-	-	-	Y	-
7	DTXSID5020491	4-(Dimethylamino)azobenzene	Y	Y	Y	Y	Y	Y	Y
8	DTXSID6020511	3,3'-Dimethylbenzidine dihydrochloride	Y	Y	Y	Y	Y	Y	Y
9	DTXSID6021082	C.I. Acid Orange 10	Y	-	-	-	Y	Y	-
10	DTXSID1021118	Phenazopyridine hydrochloride	Y	Y	-	Y	Y	Y	-
11	DTXSID4021135	C.I. Solvent Yellow 14	Y	Y	Y	-	Y	Y	Y
12	DTXSID9021213	SX purple	Y	-	-	Y	Y	Y	-
13	DTXSID8021224	C.I. Acid Red 114	Y	Y	Y	Y	Y	Y	Y
14	DTXSID8021228	Ponceau MX	Y	Y	Y	Y	Y	Y	Y
15	DTXSID7021231	Ponceau 3R	-	Y	-	Y	Y	Y	-
16	DTXSID2021232	Amaranth	Y	-	-	Y	Y	Y	-
17	DTXSID6021450	C.I. Disperse Yellow 3	Y	Y	Y	Y	Y	Y	Y
18	DTXSID1021455	FD&C Yellow 5	Y	-	-	Y	Y	Y	-
19	DTXSID6021456	FD&C Yellow 6	Y	-	-	Y	Y	Y	-
20	DTXSID9022815	Evans blue	Y	-	-	Y	-	Y	-
21	DTXSID4022816	C.I. Direct Red 28	Y	-	-	Y	-	Y	-
22	DTXSID5024059	3,3'-Dimethylbenzidine	Y	Y	Y	Y	Y	Y	Y
23	DTXSID1024415	C.I. Acid Black 1, disodium salt	Y	-	-	Y	Y	Y	-

Are there azo dye mass spectra?

- [MASSPECDB: MassBank Reference Spectra Collection](#)
- [MASSPECDB: MassBank.EU Collection: Special Cases](#)
- [MASSPECDB: Mycotoxins from MassBank.EU](#)
- [MASSPECDB: National Environmental Methods Index](#)
- [MASSPECDB: SWGDRUG Mass Spectral Library Chemical Collection](#)
- [MASSPECDB: Thermo's n](#)
- [MASSPECDB: Wiley Regi](#)
- [MASSPECDB|NORMAN:l](#)

DTXSID	PREFERRED_NAME	MASSBANK	NEMILIST	MZCLOUD	WRTMSD	INDOORCT16
DTXSID1020069	o-Aminoazotoluene	-	-	Y	-	-
DTXSID8020123	Azobenzene	-	Y	Y	-	Y
DTXSID5020491	4-(Dimethylamino)azobe	-	Y	Y	-	-
DTXSID4021135	C.I. Solvent Yellow 14	-	-	Y	-	-
DTXSID6021450	C.I. Disperse Yellow 3	-	-	Y	-	-
DTXSID1021455	FD&C Yellow 5	-	-	Y	-	-
DTXSID5024059	3,3'-Dimethylbenzidine	Y	Y	Y	-	-
DTXSID6024460	4-Aminoazobenzene	Y	Y	Y	-	-
DTXSID3025091	3,3'-Dimethoxybenzidine	Y	Y	Y	Y	-
DTXSID5040706	C.I. Solvent Orange 7	-	-	Y	-	-
DTXSID3041742	C.I. Solvent Red 23	Y	-	Y	-	-
DTXSID8041743	Scarlet red	Y	-	Y	-	-
DTXSID1042154	Methyl red	-	-	Y	-	-
DTXSID1059238	N-Phenyl-4-(phenylazo)a	-	-	Y	-	-
DTXSID7062536	Benzenamine, 4-[(4-nitro	-	-	Y	-	-
DTXSID9066883	C.I. Disperse Brown 1	-	-	Y	-	-
DTXSID2020183	Black PN	-	-	-	-	-
DTXSID7020186	C.I. Direct Blue 15	-	-	-	-	-
DTXSID3020201	C.I. Direct Brown 95	-	-	-	-	-
DTXSID0020224	Chocolate Brown HT	-	-	-	-	-

Azo dyes listed in “water” lists

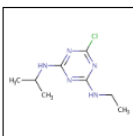
- [WATER: California Water Boards Additive Information](#)
- [WATER: Drinking Water Suspects, KWR Water, Netherlands](#)
- [WATER: EPA Drinking Water Treatability Database](#)
- [WATER: First Unregulated Contaminant Monitoring Rule](#)
- [WATER: Fourth Unregulated Contaminant Monitoring Rule](#)
- [WATER: National Recommended Water Quality Criteria - Human Health Criteria Table](#)
- [WATER: Regional Monitoring Program for Water Quality in San Francisco Bay](#)
- [WATER: Second Unregulated Contaminant Monitoring Rule](#)
- [WATER: STOFF-IDENT Database of Water-Related Substances](#)
- [WATER: Surfactant Suspect List from EI and UBA](#)
- [WATER: Surfactants Screened in Swiss Wastewater 2014](#)
- [WATER: Third Unregulated Contaminant Monitoring Rule](#)
- [WATER: Univ. Athens Surfactant and Suspect List](#)
- [WATER: USGS List of Chemicals](#)
- [WATER|EPA: Chemicals in hydraulic fracturing fluids Table H-2](#)
- [WATER|EPA: Chemicals associated with hydraulic fracturing](#)
- [WATER|EPA: Chemical Contaminants - CCL 4](#)
- [WATER|EPA: Drinking Water Standard and Health Advisories Table](#)
- [WATER|NORMAN: Extended Drinking Water Suspect Screening List](#)
- [WATER|NORMAN: GC-HRMS target list of the Slovak Water Research Institute](#)
- [WATER|NORMAN: Wastewater Suspect List based on Swedish Process](#)

DTXSID	PREFERRED_NAME	STOFFIDENT	EPAHFR	KWRSJERPS	KEMIWWSUS
DTXSID6021456	FD&C Yellow 6	-	Y	Y	Y
DTXSID1020069	o-Aminoazotoluene	-	-	Y	-
DTXSID8020123	Azobenzene	Y	-	Y	-
DTXSID9021213	SX purple	-	-	Y	-
DTXSID5024059	3,3'-Dimethylbenzidine	-	-	Y	-
DTXSID4024436	Allura Red C.I. 16035	-	-	Y	-
DTXSID6024460	4-Aminoazobenzene	Y	-	Y	-
DTXSID3025091	3,3'-Dimethoxybenzidine	Y	-	Y	-
DTXSID7041463	3,3'-Dimethyl-4,4'-diaminodiphenylmethane	Y	-	Y	-
DTXSID1052618	3-Hydroxy-2-naphthol	Y	-	Y	-
DTXSID60865718	N-Ethyl-N-(2-(1-(2-methylphenyl)ethyl)phenyl)amine	Y	-	Y	-
DTXSID2021232	Amaranth	-	Y	-	-
DTXSID1021455	FD&C Yellow 5	-	Y	-	Y
DTXSID5050395	C.I. Solvent Red 26	-	Y	-	-
DTXSID2020183	Black PN	-	-	-	-
DTXSID7020186	C.I. Direct Blue 15	-	-	-	-
DTXSID3020201	C.I. Direct Brown 95	-	-	-	-
DTXSID9020324	Chocolate Brown HT	-	-	-	-
DTXSID5020491	4-(Dimethylamino)azobenzene	Y	-	-	-
DTXSID6020511	3,3'-Dimethylbenzidine	-	-	-	-
DTXSID6021082	C.I. Acid Orange 10	-	-	-	-

LINKAGES OUTBOUND and INBOUND

Increasingly important identifier

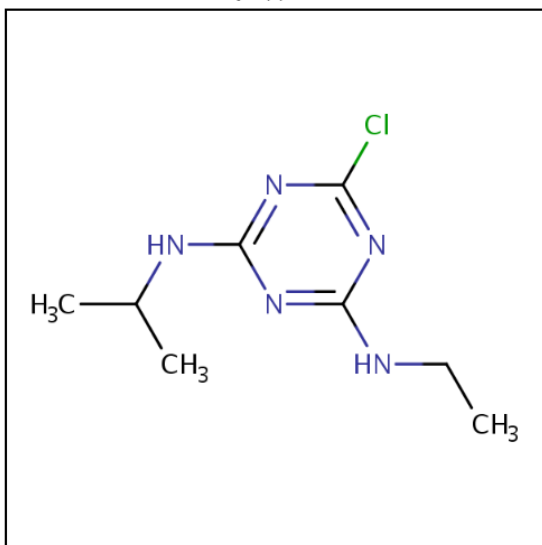
The DTXSID



Atrazine

1912-24-9 **DTXSID9020112**

Searched by Approved Name.



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:** C₈H₁₄ClN₅  Mol File  Find All Chemicals

 **Average Mass:** 215.69 g/mol  Isotope Mass Distribution

 **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:** CCNC1=NC(NC(C)C)=NC(Cl)=N1

In-links from various sources

Wikipedia article for Cannabidivarin. The article text includes: "Cannabidivarin (CBDV) is a non-psychoactive cannabinoid found in Cannabis. It is a homologue of cannabidiol (CBD), with the side-chain shortened by two methylene bridges (CH₂ units). Plants with relatively high levels of CBDV have been reported in local populations of *C. indica* (= *C. sativa* ssp. *indica* var. *Afghanistanica*) from northwest India, and in hashish from Nepal (1992). CBDV has anticonvulsant effects (1). It was identified for the first time in 1999 by Vothler et al (2). Similarly to CBD, it has seven double bond isomers and 20 stereoisomers (see Cannabidivarin double bond isomers and their stereoisomers). It is not listed by the Convention on Psychotropic Substances. It is being actively investigated as GPR42 agonist because of demonstrated neurochemical profile (3), previously observed anti-epileptic and anti-convulsive action (4) GW has been investigated for its potential as a treatment for epilepsy (5)."

Wikipedia

AOPWiki interface showing a table of AOPs and a list of stressors.

AOP Name	Evidence
GNRH pulse disruption leading to mammary adenomas and carcinomas in the SD rat.	
GNRH pulse disruption leading to pituitary adenomas and carcinomas in the SD rat.	
D1 protein blockage leading to photosystem II (PSII)-inhibition associated growth reduction	High

Events Including This Stressor

Chemical Table

User term	DTXID	Preferred name	Casrn	jchem_inchi_key	indigo_inchi_key
atrazine	DTXSID0020112	Atrazine	1912-24-0	MXWJVTOORXGIU-LHFFFAOYSA-N	MXWJVTOORXGIU-LHFFFAOYSA-N

AOP Wiki

PubChem interface for Atrazine (Compound). The page shows various identifiers and a table of contents.

PubChem Atrazine (Compound)

2.3.7 UNII

2.3.8 DSSTox Substance ID

2.3.9 Wikipedia

2.3.10 Shipping Name/ Number DOT/UN/NA/IMO

PubChem

MassBank interface showing mass spectrum and chemical structure for 6-CHLORO-N-ETHYL-N*-(1-METHYLETHYL)-1,3,5-TRIAZINE-2,4-DIAMINE: EI-B: MS.

6-CHLORO-N-ETHYL-N*-(1-METHYLETHYL)-1,3,5-TRIAZINE-2,4-DIAMINE: EI-B: MS

Mass Spectrum

Abundance

1000

800

600

400

200

0.000

50.00

Chemical Structure

MassBank

UniChem interface showing search results for Atrazine.

UniChem

Search results table:

Source Name	Chemical Formula	Chemically Assigned	LR	Pubchem ID	Standard InChIKey
chembl	CHEMBL15063	Yes		298349	MXWJVTOORXGIU-UHFFFAOYSA-N
pub	ATZ	Yes		298349	MXWJVTOORXGIU-UHFFFAOYSA-N
chembl	15930	Yes		298349	MXWJVTOORXGIU-UHFFFAOYSA-N
surechembl	SURECHEMBL21045984	Yes		298349	MXWJVTOORXGIU-UHFFFAOYSA-N
drugbank	DB07392	Yes		298349	MXWJVTOORXGIU-UHFFFAOYSA-N
kegg_ligand	C06551	Yes		298349	MXWJVTOORXGIU-UHFFFAOYSA-N
zinc	ZINC00003078958	Yes		298349	MXWJVTOORXGIU-UHFFFAOYSA-N
zinc	ZINC03078958	No	12-MAR-2012	298349	MXWJVTOORXGIU-UHFFFAOYSA-N
emolecules	495715	Yes		298349	MXWJVTOORXGIU-UHFFFAOYSA-N
lm	090D43859892FBF32B48773C6855B40	Yes		298349	MXWJVTOORXGIU-UHFFFAOYSA-N

UniChem



Main page
Community portal
Project chat
Create a new Item
Create a new Lexeme
Recent changes
Random Item
Query Service
Nearby
Help
Donate

Tools
What links here
Related changes
Special pages
Permanent link
Page information
In Wikipedia
Add links

English Not logged in Talk Contributions Create account Log in

Project page Discussion

Read Edit View history

Search Wikidata

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)

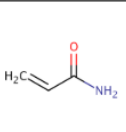
Description	This DTXSID is the DSSTox substance identifier used in the Environmental Protection Agency CompTox Dashboard.
Data type	External identifier
Domain	chemical substance (Q79529)
Example	benzene (Q2270) → DTXSID3039242
Planned use	Adding DTXSIDs to @wikidata using a bot or possible Mix&Match, based on InChIKey matches and this CCZero data on Figshare: https://figshare.com/articles/Mapping_file_of_InChIStrings_InChIKeys_and_DTXSIDs_for_the_EPA_CompTox_Dashboard/3578313/1 .
Formatter URL	https://comptox.epa.gov/dashboard/\$1

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 \(Q26701395\)](#)). 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

79-06-1 | DTXSID5020027

Searched by Approved Name.

General	Toxicology	Publications	Analytical	Prediction
EPA Substance Registry Service Household Products Database Chemical Entities of Biological Interest (ChEBI) PubChem Chempider CPCat DrugBank HMDB Wikipedia MSDS Lookup ChEMBL Chemical Vendors CalEPA OEHHA NIOSH Chemical Safety Cards ToxPlanet ACS Reagent Chemicals Wikidata ChemHat: Hazards and Alternatives Toolbox	ACToR DrugPortal CCRIS ChemView CTD eChemPortal Gene-Tox HSDB ToxCast Dashboard 2 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	Toxline Environmental Health Perspectives NIEHS 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	FOR-IDENT NEMI: National Environmental Methods Index RSC Analytical Abstracts Tox21 Analytical Data MONA: MassBank North America mzCloud NIST NIST IR Spectrum NIST NIST MS Spectrum ECOTOX MassBank NEMI: National Environmental Methods Index NIST NIST Antoine Constants IR Spectra on PubChem NIST NIST Kovats Index values Protein DataBank	2D NMR HSQC/HMBC Prediction Carbon-13 NMR Prediction Proton NMR Prediction ChemRTP Predictor LSERD

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 [CompTox Chemical Dashboard](#) for more information on this chemical.

Modernizing Public Hearings for WQS Reviews

The document below suggests how states and authorized tribes can conduct online public hearings in lieu of in-person public hearings, consistent with federal public hearing requirements.

- [Modernizing Public Hearings for Water Quality Standard Decisions Consistent with 40 CFR 25.5 \(PDF\)](#) (31 pp, 686 K)

Show entries

State	Parameter (the name used by the state)	Application	Criteria Magnitude
<input type="text" value="Search this column."/>	<input type="text" value="Search this column."/>	<input type="text" value="Search this column."/>	<input type="text" value="Search this column."/>
Alaska	atrazine Source Page 5	drinking water MCL (water supply (drinking, culinary and food processing); contact recreation) (<i>Human Health</i>)	0.0030 mg/l
Arizona	atrazine Source Page 20	Domestic Water Source (DWS) (<i>Human Health</i>)	3 µg/l
Arizona	atrazine Source Page 20	Full-Body Contact (FBC) (<i>Human Health</i>)	32667 µg/l
Arizona	atrazine Source Page 20	Partial-Body Contact (PBC) (<i>Human Health</i>)	32667 µg/l
California Region 1 - North Coast	atrazine Source Page 47	municipal or domestic supply (<i>Human Health</i>)	0.0030 mg/l
California Region 2 - San Francisco Bay	atrazine Source Page 54	municipal supply	0.0030 mg/l
California Region 3 - Central Coast	atrazine Source Page 48	domestic or municipal supply	0.0030 mg/l
California Region 4 - Los Angeles	atrazine Source Page 135	municipal and domestic water supply (<i>Human Health</i>)	0.001 mg/l
California Region 9 - San Diego	atrazine Source Page 162	municipal or domestic supply (<i>Human Health</i>)	0.0030 mg/l
Colorado	atrazine Source Page 31	drinking water supply (<i>Human Health</i>)	3 µg/l

Showing 1 to 10 of 41 entries

Previous Next

[↑ Top of Page](#)

New Outlinks of Interest

PubChem Chemical Vendors

PUBCHEM > ATRAZINE > CHEMICAL VENDORS

CID 2256

Atrazine

Chemical Vendors

69 Substances

Yuhao Chemical

PubChem SID: [355047054](#) Purchasable Chemical: [LT4922](#)

PubChem SID: [347737622](#) Purchasable Chemical: [LT6957](#)

Achemo Scientific Limited

PubChem SID: [252453703](#) Purchasable Chemical: [AC-11427](#)

Sigma-Aldrich

PubChem SID: [329753681](#) Purchasable Chemical: [31212_SIAL](#)

PubChem SID: [329756651](#) Purchasable Chemical: [45330_SIGMA](#)

PubChem SID: [24871790](#) Purchasable Chemical: [48187_SUPELCO](#)

PubChem SID: [24872608](#) Purchasable Chemical: [49085_SUPELCO](#)

PubChem SID: [329769969](#) Purchasable Chemical: [90935_SIAL](#)

PubChem SID: [329823655](#) Purchasable Chemical: [PS380-250MG_SUPELCO](#)

PubChem SID: [24899206](#) Purchasable Chemical: [PS380_SUPELCO](#)

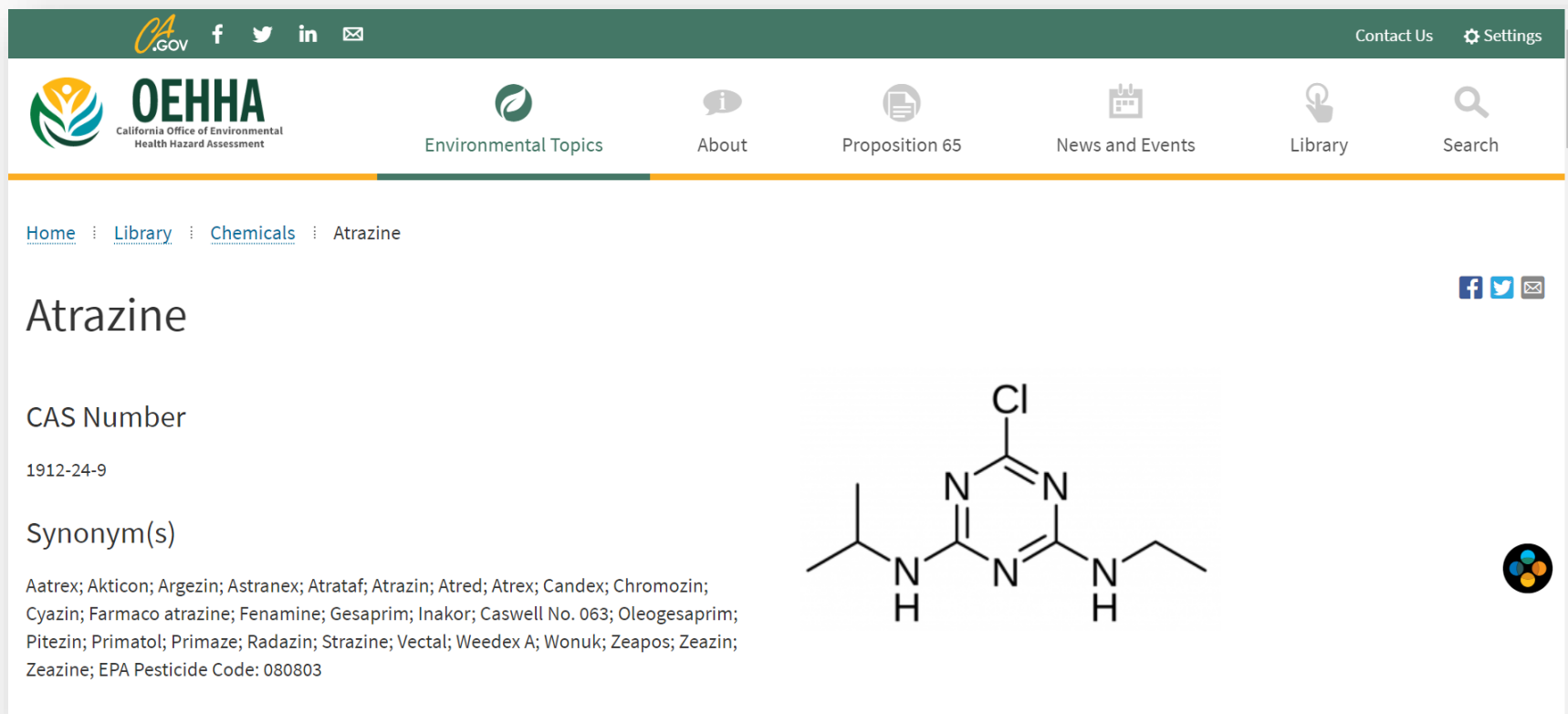
ZINC

PubChem SID: [256808431](#) Purchasable Chemical: [ZINC3078958](#)

Acadechem

PubChem SID: [321908354](#) Purchasable Chemical: [ACDS-021206](#)


New Outlinks of Interest California EPA OEHHA





The screenshot shows the OEHHA website interface. At the top, there is a navigation bar with social media icons (CA.GOV, Facebook, Twitter, LinkedIn, Email) and links for Contact Us and Settings. Below this is a main menu with icons for Environmental Topics, About, Proposition 65, News and Events, Library, and Search. The breadcrumb trail reads: Home > Library > Chemicals > Atrazine. The page title is "Atrazine". To the right of the title are social media icons for Facebook, Twitter, and Email. Below the title, the "CAS Number" is listed as 1912-24-9. The "Synonym(s)" section lists: Aatrex; Akticon; Argezin; Astranex; 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. To the right of the text is the chemical structure of Atrazine, which is a 1,3,5-triazine ring with a chlorine atom at position 4, an isopropylamino group at position 6, and an ethylamino group at position 2.


CA.GOV f t in ✉


Contact Us ⚙ Settings


 **OEHHA**
California Office of Environmental
Health Hazard Assessment


 Environmental Topics

 About




 Proposition 65

 News and Events

 Library

 Search

[Home](#) > [Library](#) > [Chemicals](#) > Atrazine


Atrazine

CAS Number

1912-24-9

Synonym(s)

Aatrex; Akticon; Argezin; Astranex; 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

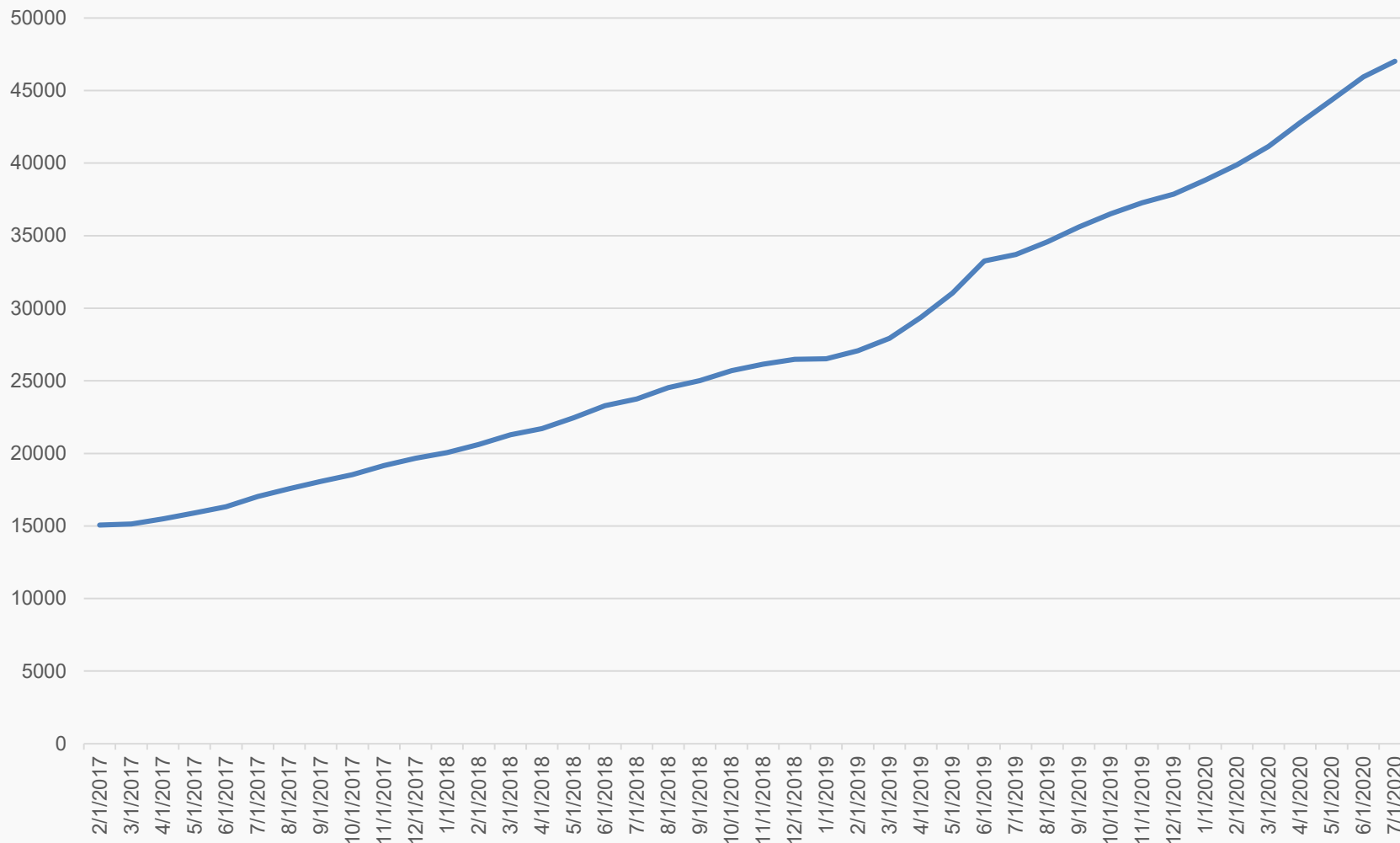
CC(C)Nc1nc(Cl)n(CCN)c1

CONTRIBUTING
to
DATA QUALITY

Ongoing Data Review


Thanks to our curators!

Cumulative Manual



- View the level of curation for any chemical
- If you see any issues let us know

Record Information

 **Citation:** U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. <https://comptox.epa.gov/dashboard/DTXSID3031864> (accessed July 23, 2020), Perfluorooctanesulfonic acid

Data Quality:

Level 1: Expert curated, highest confidence in accuracy and consistency of unique chemical identifiers

Level 2: Expert curated, unique chemical identifiers using multiple sources

Level 3: Programmatically curated from high quality EPA source, unique chemical identifiers have no conflicts in ChemID and PubChem

Level 4: Programmatically curated from ChemID, unique chemical identifiers have no conflicts in PubChem

Level 5: Programmatically curated from ACToR or PubChem, unique chemical identifiers with low confidence, single public source


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.

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

- 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”

Download Experimental Data ▾

Source	Result
Danish_EPA_SCPFAS_Report_2015	
NCCT_Physchem	7.03
NCCT_Physchem	5.50
Rayne et al. J. Env. Sci. and Health Part A, (2009) 44(12):1145-1199	4.30

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 
reCAPTCHA
[Privacy](#) - [Terms](#)

Submit






>400 Comments to Date

Cleaning chemistry one at a time

Crowdsourced Comments

25 ▾

Search query

Chemical	Structure	Date	Comment	Resolution
Oxazole, 2-ethyl-4,5-dimethyl-		2020-07-22	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 507360 FEMA 3672 MFCD00036664 Barrie	Resolved
4-Decenoic acid, ethyl ester, (4E)-		2020-07-22	Add names Ethyl (4E)-4-decenoate (uninverted CAS name) Ethyl (E)-dec-4-enoate (IUPAC) FEMA 3642 REAXYS/BRN 1770966 WLN 6U3VO2 &&E or trans Form REACH 278-509-4 (ex EINECS) PubChem CID 5362583 MFCD00015574 UNII-3I89X5937N Barrie	Resolved
Hexanedioic acid, diisononyl ester	No Chemical Structure Associated with this Substance	2020-07-21	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 that there are results from toxcast/tox21) or the toxcast models. Examples are 33703-08-1 and 27178-16-1 .	Resolved
2-Pental, 5-(methylthio)-2-[(methylthio)methyl...]		2020-07-20	2,8-Dithianon-4-en-4-carboxaldehyde should be..aldehyde 2-Methylthiomethyl-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 Methialdol REAXYS/BRN is 2241044 WLN is 1S3UYVH1S1 Barrie	Resolved
Dipentyl 2-hydroxybutanedioate		2020-07-20	well known as Dipentyl malate WLN 5OVYQ1VO5 Barrie	Resolved
Tricyclo[1.1.0.0~2,4~]tetraphosphane		2020-07-20	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.	Resolved

PROTOTYPES
in
PROGRESS

Proof-of-Concept: Structure/ Substructure/Similarity Searches

AADashboard

atrazine

Search



Select properties to predict

T.E.S.T. 18 OPERA Search

- Exact
- Substructure
- Similarity
- Molecular Formula
- Molecular Weight

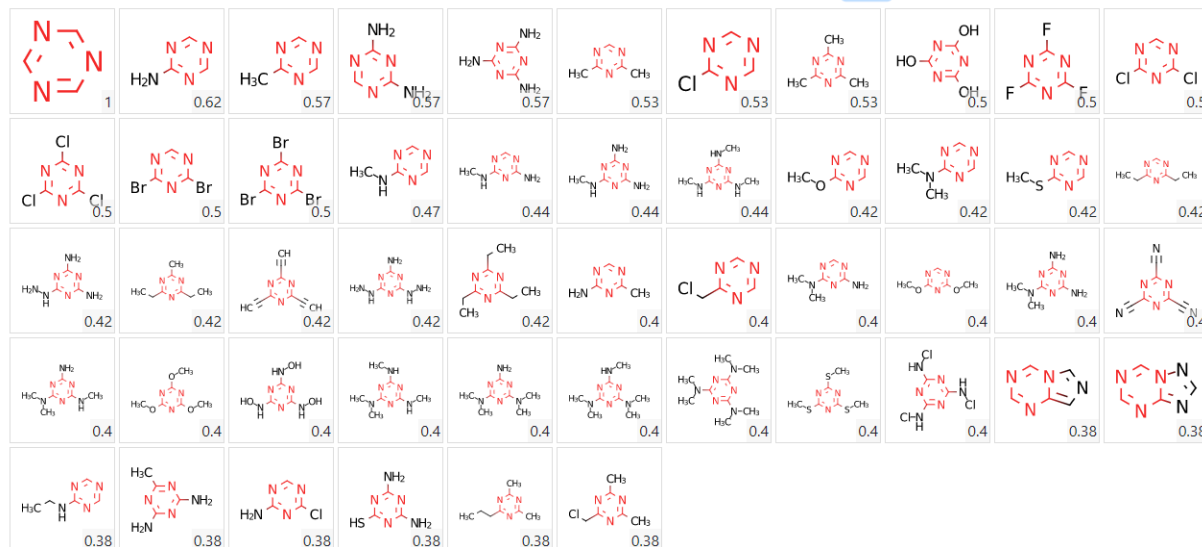
Filter by elements (enter comma separated list e.g. C,F,H) include

Filter by elements (enter comma separated list e.g. C,F,H) exclude

Search result 2540

Show Isotopically Labeled Charged Salts or Mixtures

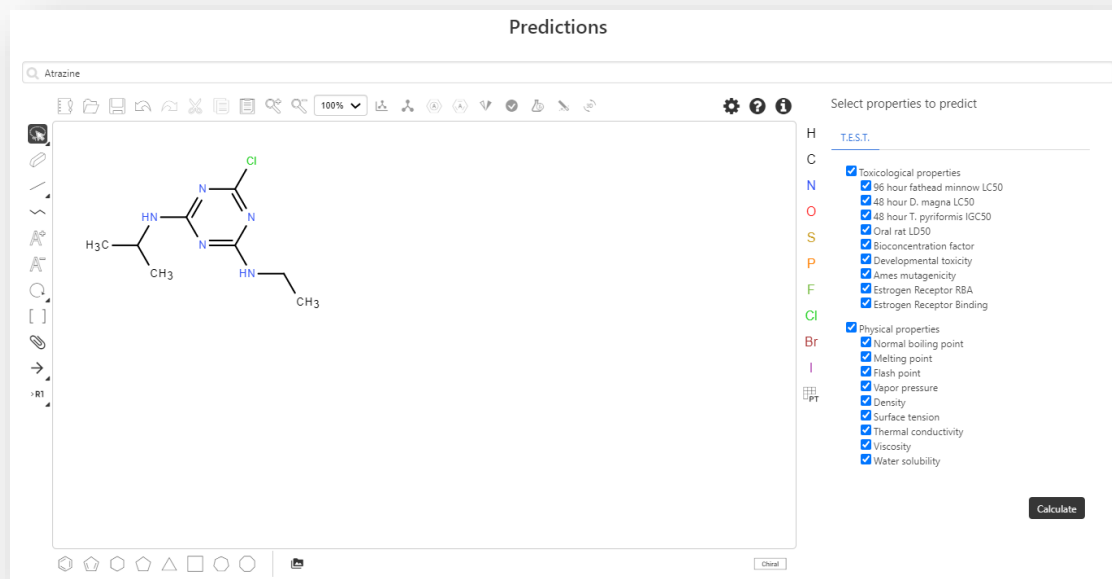
Sort Similarity



Search result 2540

Show Isotopically Labeled


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




“RapidTox” *Proof-of-Concept*



**CompTox
Chemicals
Dashboard**



**Aggregated
Publicly Available
Chemical Data
ACToR**



**ToxCast
Dashboard
High-throughput
screening data**



EDSP21 Dashboard
High-throughput screening
and exposure estimates for
evaluating chemicals for
potential endocrine activity



RapidTox
Decision support workflows
to integrate chemistry,
toxicity, and exposure
information



Downloadable Data

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.




Alternatives Assessment Dashboard - a foundation technology

Clean Technologies and Environmental Policy (2020) 22:441–458
<https://doi.org/10.1007/s10098-019-01795-w>

ORIGINAL PAPER



An automated framework for compiling and integrating chemical hazard data

Leora Vegosen^{1,2} · Todd M. Martin² 

Received: 3 October 2019 / Accepted: 13 December 2019 / Published online: 21 January 2020

© This is a U.S. Government work and not under copyright protection in the US; foreign copyright protection may apply 2020

Now: "Hazard Comparison Dashboard"

Hazard Comparison Dashboard

Hazard Comparison ▾ None ▾ Export ▾ 21 / 21 🔍 📄

Legend: VH - Very High, H - High, M - Medium, L - Low, I - Inconclusive **Authoritative**, Screening, QSAR Model

CAS Name	Human Health Effects															Ecotoxicity		Fate	
	Acute Mammalian Toxicity			Carcinogenicity	Genotoxicity Mutagenicity	Endocrine Disruption	Reproductive	Developmental	Neurotoxicity		Systemic Toxicity		Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation
	Oral	Inhalation	Dermal						Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure							
56-23-5 Carbon tetrachloride	H	H	H	VH	L	H	M	L		H	H	H	H	H	H	VH	M	H	I
108-90-7 Chlorobenzene	M	M	I	I	H	L	L	L	H		H	H	I	H	H	VH	H	H	L
542-88-1 bis(Chloromethyl) ether	M	VH	H	VH	I	L	I	I		I	H	I	I	VH	I	L	I	H	L
7782-50-5 Chlorine	VH	H	I	I	I		L	L			H	M	I	H	H	VH	VH	H	L
123-73-9 (E)-Crotonaldehyde	H	VH	H	VH	H	H	I	I	I	I	M	M	I	H	VH	VH	VH	L	L

Filters
 Structure
 Products

• Watch this space....

***WHAT'S THE
NEXT BIG
CHANGE?***

- 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

- 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 early days of the dashboard

<https://jcheminf.springeropen.com/articles/10.1186/s13321-017-0247-6>

Williams et al. *J Cheminform* (2017) 9:61
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. Williams^{1*} , Christopher M. Grulke¹, 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

The many years of data curation...

<https://www.sciencedirect.com/science/article/pii/S2468111319300234>

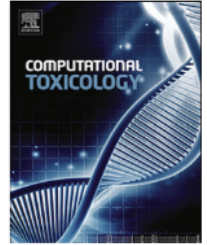
Computational Toxicology 12 (2019) 100096



Contents lists available at ScienceDirect

Computational Toxicology

journal homepage: www.elsevier.com/locate/comtox



EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research



Christopher M. Grulke^a, Antony J. Williams^a, Inthirany Thillanadarajah^b, Ann M. Richard^{a,*}

- We owe a great debt to the curators who have invested efforts over ~20 years

Downloadable Data Will Be Updated


 United States
 Environmental Protection
 Agency

[Home](#)
[Advanced Search](#)
[Batch Search](#)
[Lists](#)
[Predictions](#)
[Downloads](#)



Chemistry Dashboard

Aa ▼ Aa Aa ▲

Downloads

[DSSTox Identifier to PubChem Identifier Mapping File](#)

Posted: 11/14/2016

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

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

[DSSTox identifiers mapped to CAS Numbers and Names File](#)

Posted: 11/14/2016

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

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

- 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...)