

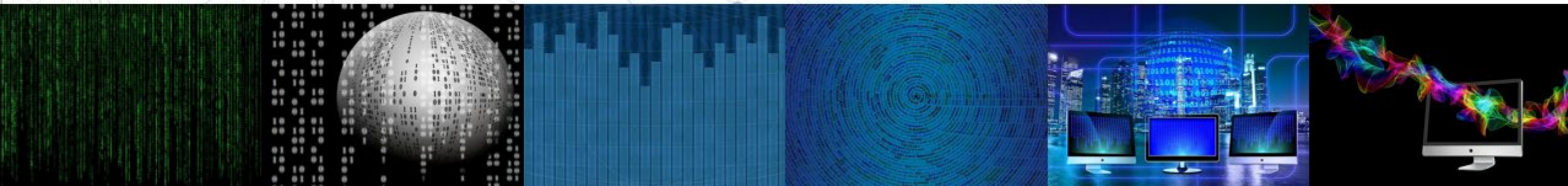


Welcome!

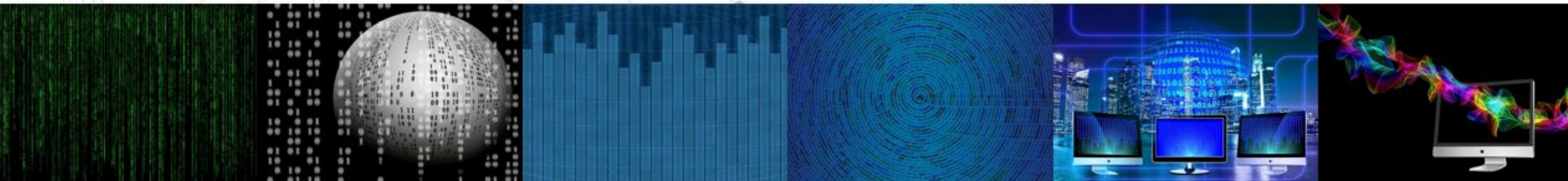
This Session will Begin at 2:00 pm Eastern US Time

**HOW TO PLACE YOUR RESEARCH QUESTIONS
OR RESULTS INTO THE CONTEXT OF THE “LEGACY”
TOXICOLOGY DATA ?**

Antony Williams - US Environmental Protection Agency



- All participants are muted to enable the speaker to present without interruption.
- Please rename yourself and designate Full Name and Affiliation.
- Use the reaction icon at the bottom of your screen to raise your hand.
- This meeting will be recorded, and posted on the [@tamusuperfund](https://superfund.tamu.edu/big-data-series-2021/) website <https://superfund.tamu.edu/big-data-series-2021/> in the coming weeks.



How to Place Your Research Question or Results into the Context of Legacy Data

Antony John Williams

williams.antony@epa.gov

Center for Computational Toxicology and Exposure, US-EPA, RTP, NC

My background...

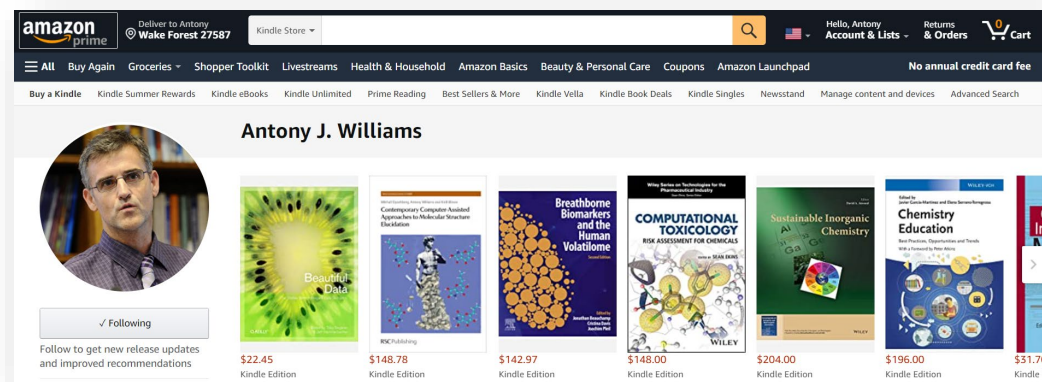
- Worked in
 - Government lab as postdoc
 - Academia as NMR Facility Manager
 - Fortune 500 Company as NMR Tech Leader
 - Small start-up company as product manager, marketing manager, Chief Science Officer
 - Consultant – chemistry informatics industry
 - Company owner – created ChemSpider
 - Royal Society of Chemistry (bought ChemSpider)
 - US-EPA – cheminformatician and “connector”

Who am I today?

<https://orcid.org/0000-0002-2668-4821>



- Computational chemist at the US-EPA – **scientist**
- Responsibility for cheminformatics projects, internal & external collaborations, “product marketing” – **cheminformatician**
- Work with a team of people developing software solutions – “**product & project manager**”
- Scientific publications, books, blogger – **author**; I am @ChemConnector – **social networker**



Antony Williams

ORCID iD

<https://orcid.org/0000-0002-2668-4821>

Print view

Also known as

ChemConnector, ChemSpiderman, Tony Williams

Country

United States

Keywords

NMR, Computer-assisted Structure Elucidation, Chemistry, ChemSpider, Cheminformatics, Open PHACTS, PharmaSea, Open Science, Computational Toxicology

Other IDs

Scopus Author ID: 55258539900
US EPA VIVO: [williams.antony](#)
ResearcherID: C-3089-2009

- CompTox - Computational Toxicology
- DSSTox - Distributed Structure Searchable Toxicity DB
- CASRN - Chemical Abstracts Registry Number
- InChI - International Chemical Identifier
- QMRF – QSAR Model Report Format
- ToxVal - Toxicity Value Database
- OPERA - OPEn structure–activity

Relationship App

- TEST - Toxicity Estimation Software Tool
- ToxCAST - Toxicity Forecaster
- SDF - Structure data file

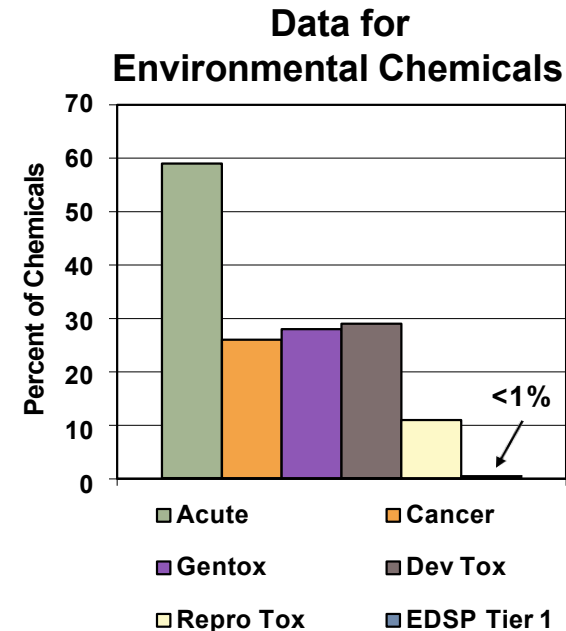
- A *very short* overview of cheminformatics focused on
 - Chemical identifiers and some associated challenges
 - Molecular fingerprints
 - Molecular similarity
 - Structure-based modeling (QSAR/QSPR/QSUR)
- An overview of the CompTox Chemicals Dashboard and how it can help to:
 - Search, source, visualize and download data for singleton or thousands of chemicals
 - Perform real-time prediction calculations and read-across
 - Navigate into dozens of other online resources that contain additional data

Problem: Too Many Chemicals and Too Few Resources

- Fast characterization of human and ecological risk posed by existing and emerging chemicals is a critical challenge
- Chemistry never stops. But there is sparse and distributed data...



CAS REGISTRY® contains more than **171 million unique organic and inorganic chemical substances**, such as alloys, coordination compounds, minerals, mixtures, polymers and salts, and more than 68 million protein and DNA sequences



Modified from Judson *et al.*, EHP 2010

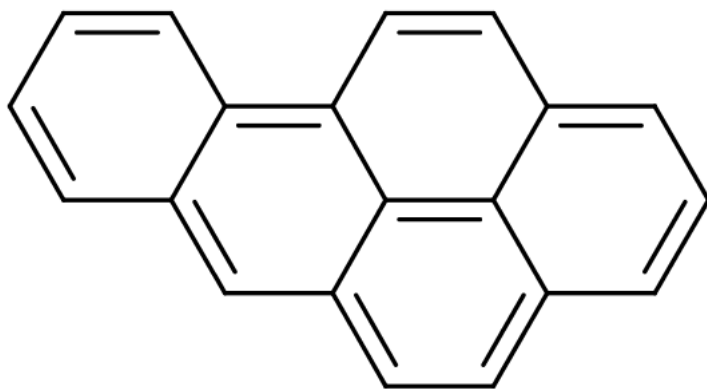
- Develop a “first-stop-shop” for environmental chemical data to support EPA and partner decision making:
 - **Centralized location** for relevant chemical data
 - Chemistry, exposure, hazard and dosimetry
 - Combination of existing data and predictive models
 - Publicly accessible, periodically updated, curated
- Easy access to data improves efficiency and ultimately accelerates chemical risk assessment

Cheminformatics and the Dashboard

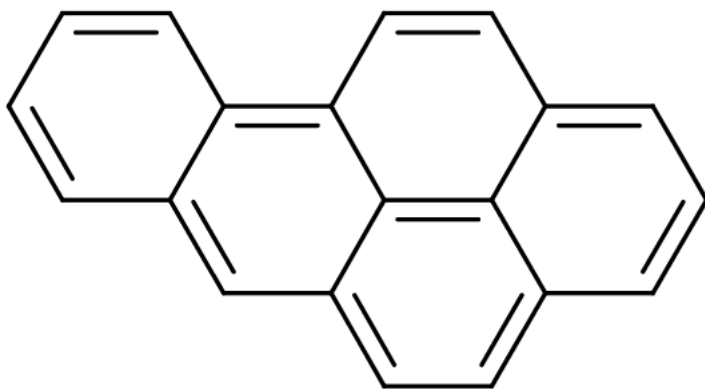


- Cheminformatics is the application of computer science and informatics-based approaches to:
 - Represent chemical structures, substances and reactions
 - Store chemistry-related data
 - Search for chemistry related data
 - Model data sets to provide predictive capabilities
 - Visualize and analyse chemistry related data
- The US-EPA uses cheminformatics (and bioinformatics) to manipulate, integrate, store, model and deliver access to our data. The CompTox Chemicals Dashboard is built on a solid cheminformatics foundation

Types of Chemical Identifiers



- Structural Identifiers
- The visual depiction
- Multiple electronic formats
- InChI (Key): FMMWHPNWAFFZXNH-UHFFFAOYSA-N
- Common Name: Benzo(a)pyrene
- Systematic Name: Benzo[*pqr*]tetraphene
- CAS Registry Number(s) : 50-32-8
- Lots of other “common names and trade names”



INTRINSIC PROPERTIES

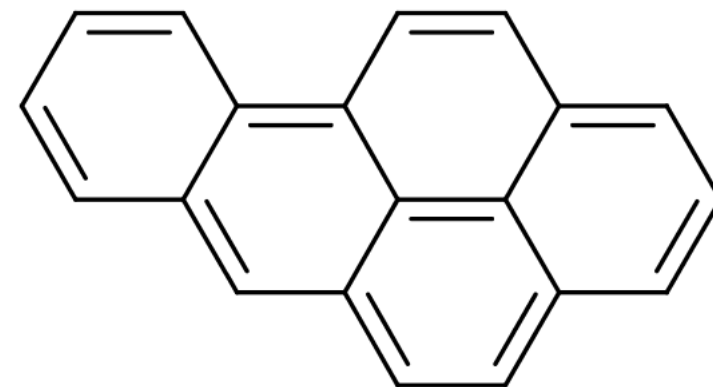
- Formula : $C_{20}H_{12}$
- Molecular weight: 252.316 g/mol
- Monoisotopic Mass: 252.093900 g/mol

MEASURED PROPERTIES

- LogKow 6.13
- Melting Pt 177°C
- Boiling Pt 485°C
-and many more

How to Store a Chemical Structure

- Multiple approaches:
 - Names and identifiers
 - 2D or 3D structure “molfile”



```
Mrv1533009301517202D
  0  0  0      0  0      999 V3000
M  V30 BEGIN CTAB
M  V30 COUNTS 20 24 0 0 0
M  V30 BEGIN ATOM
M  V30 1 C 5.3801 0 0 0
M  V30 2 C 6.9201 0 0 0
M  V30 3 C 7.6901 -1.33 0 0
M  V30 4 C 9.2302 -1.33 0 0
M  V30 5 C 10.0003 -2.67 0 0
M  V30 6 C 9.2302 -4.0001 0 0
M  V30 7 C 7.6901 -4.0001 0 0
M  V30 8 C 6.9201 -5.3301 0 0
M  V30 9 C 5.3801 -5.3301 0 0
M  V30 10 C 4.6201 -4.0001 0 0
M  V30 11 C 5.3801 -2.67 0 0
M  V30 12 C 6.9201 -2.67 0 0
M  V30 13 C 4.6201 -1.33 0 0
M  V30 14 C 3.0801 -1.33 0 0
M  V30 15 C 2.31 -2.67 0 0
M  V30 16 C 3.0801 -4.0001 0 0
M  V30 17 C 0.77 -2.67 0 0
M  V30 18 C 0 -1.33 0 0
M  V30 19 C 0.77 0 0 0
M  V30 20 C 2.31 0 0 0
M  V30 END ATOM
M  V30 BEGIN BOND
M  V30 1 2 1 2
M  V30 2 1 1 13
M  V30 3 1 2 3
M  V30 4 2 3 4
M  V30 5 1 3 12
M  V30 6 1 4 12
```

- SMILES:
 - c1cc2c3ccc4ccccc5ccc(cc2cc1)c3c45
 - C1=CC2=CC3=CC=C4C=CC=C5C=CC(=C2C=C1)C3=C45
 - and many other variants....
- InChI=1S/C20H12/c1-2-7-17-15(4-1)12-16-9-8-13-5-3-6-14-10-11-18(17)20(16)19(13)14/h1-12H
- InChIKey: FMMWHPNWAFFZXNH-UHFFFAOYSA-N

If We Database Chemical Structures...

- ...then we can search the dataset by inherent **structural** properties
 - Formula
 - Mass
 - Substructure
 - Structural similarity
- ...we can **integrate** other info into the database for retrieval
- ...available data, both experimental and predicted, is a click away
- ...data can be downloaded, distributed and shared
- ...linking out to other resources enabled by adopting specific standards
- ...structure collections, with associated data, are available for modeling

CompTox Chemicals Dashboard

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



Home

Advanced Search

Batch Search

Lists

Predictions

Downloads

875 Thousand Chemicals

SEARCH

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

Identifier subsetting search

See what people are saying: read the dashboard comments! Cite the Dashboard Publication click here

Chemicals

Product/Use Categories

Assay/Gene

Latest News

Read more news

List of Terpenes added to Dashboard

19th, 2019 at 12:28:28 AM

Chemical list related to terpenes found in vape has been added to the dashboard and is available at: comptox.epa.gov/dashboard/chemical_lists/VAPETERPENES

Batch Search

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

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

Select Input Type(s)

Select Output Format

Download Chemical Data

Customize Results

Download

Details

Executive Summary

Properties

Env. Rate/Transport

Hazard

Acute

Exposure

Bioactivity

Similar Compounds

Genra (Beta)

Related Substances

Synonyms

Literature

Links

DTXSID	Chemical Name	Year	Title	Authors	Journal
DTXSID00000001	1,1,1-Trichloroethane	1978	Developmental treatment with ethyl alcohol: does not alter the effects of 1,1,1-trichloroethane on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000002	1,1,1-Trichloroethane	1979	Impact of Low-Dose Oral Exposure to Bisphenol A (BPA) on Juvenile and Adult Rat Reproductive Development	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000003	1,1,1-Trichloroethane	1980	Investigation of the effects of subchronic low-dose oral exposure to bisphenol A (BPA) and ethyl alcohol on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000004	1,1,1-Trichloroethane	1981	Toxicity evaluation of bisphenol A administered by gavage to Sprague-Dawley rats from gestation to adulthood	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000005	1,1,1-Trichloroethane	1982	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000006	1,1,1-Trichloroethane	1983	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000007	1,1,1-Trichloroethane	1984	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000008	1,1,1-Trichloroethane	1985	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000009	1,1,1-Trichloroethane	1986	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000010	1,1,1-Trichloroethane	1987	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000011	1,1,1-Trichloroethane	1988	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000012	1,1,1-Trichloroethane	1989	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000013	1,1,1-Trichloroethane	1990	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000014	1,1,1-Trichloroethane	1991	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000015	1,1,1-Trichloroethane	1992	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000016	1,1,1-Trichloroethane	1993	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000017	1,1,1-Trichloroethane	1994	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000018	1,1,1-Trichloroethane	1995	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000019	1,1,1-Trichloroethane	1996	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000020	1,1,1-Trichloroethane	1997	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000021	1,1,1-Trichloroethane	1998	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000022	1,1,1-Trichloroethane	1999	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000023	1,1,1-Trichloroethane	2000	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000024	1,1,1-Trichloroethane	2001	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000025	1,1,1-Trichloroethane	2002	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000026	1,1,1-Trichloroethane	2003	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000027	1,1,1-Trichloroethane	2004	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000028	1,1,1-Trichloroethane	2005	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000029	1,1,1-Trichloroethane	2006	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000030	1,1,1-Trichloroethane	2007	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000031	1,1,1-Trichloroethane	2008	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000032	1,1,1-Trichloroethane	2009	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000033	1,1,1-Trichloroethane	2010	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000034	1,1,1-Trichloroethane	2011	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000035	1,1,1-Trichloroethane	2012	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000036	1,1,1-Trichloroethane	2013	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000037	1,1,1-Trichloroethane	2014	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000038	1,1,1-Trichloroethane	2015	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000039	1,1,1-Trichloroethane	2016	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000040	1,1,1-Trichloroethane	2017	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000041	1,1,1-Trichloroethane	2018	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000042	1,1,1-Trichloroethane	2019	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000043	1,1,1-Trichloroethane	2020	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000044	1,1,1-Trichloroethane	2021	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists
DTXSID00000045	1,1,1-Trichloroethane	2022	Exposure to bisphenol A during pregnancy and lactation: effects on the development of the rat	Parsons, Lorr, Krasner	Toxicological sciences: an official journal of the Society of Toxicologists

TOX DATA

Bisphenol A

80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.

Hazard

Human

Eco

Download

Columns

Details

Executive Summary

Properties

Env. Rate/Transport

Hazard

Acute

Exposure

Bioactivity

Similar Compounds

Genra (Beta)

Related Substances

Synonyms

Literature

Links

BIOACTIVITY

Bisphenol A

80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.

Chemical Activity Summary

TOXCAST DATA

ASSAY DETAILS

AC90 (ARL 175)

Assay Endpoint Name: OT_UR_EstR04_0400

Assay Description: TSC

Gene Symbol: ESR1

Organism: Human

Tissue: Kidney

Assay Format Type: cell-based

Biological Process: Target protein stabilization

Detection Technology: Protein-fragment Complementation Analysis

Analysis Direction: positive

Intended Target Family: nuclear receptor

Description: Data from the assay component OT_UR_EstR04_0400 was analyzed into 1 assay endpoint. This assay endpoint, OT_UR_EstR04_0400, 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 of 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 related targets, this assay endpoint is associated to the "nuclear receptor" intended target family, where the subfamily is "nuclear".

ACROSS

Neighbors by: Chem-Voronoi

Filter by: InChI data

Summary Data Gap Analysis

Group: Similar

Big: Top 100

Generate Data Matrix

Chemical structure diagram showing Bisphenol A and its neighbors.

SIMILARITY

Bisphenol A

80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.

Searched with a similarity threshold of 0.8

378 of 390 chemicals visible

Download

Send to Batch Search

Similarity

Color

Order


DTXSID

Chemical structure diagram showing Bisphenol A and its similar compounds.

CompTox Chemicals Dashboard



883k Chemical Substances



United States
Environmental Protection
Agency

HomeAdvanced SearchBatch SearchLists▼PredictionsDownloads

Share▼



CompTox Chemicals Dashboard

883 Thousand Chemicals

Chemicals

Product/Use Categories

Assay/Gene

☐ 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](#).

UNITED STATES

Discover


Connect

Ask


BASIC Search

Chemicals Product/Use Categories Assay/Gene


Q Benzo(a)pyrene




Benzo(a)pyrene
DTXSID2020139




Benzo(a)pyrene diolepoxide 1
DTXSID9036779




Benzo(a)pyrene- 7,8,9-triol,7,8,9,10-tetrahydro-, (7-alpha,8-beta,9-beta)-
DTXSID00210066




Benzo(a)pyrene-1-methanol
DTXSID40235374




Benzo(a)pyrene-1,6-dione, 7-methyl-
DTXSID70229645




Benzo(a)pyrene-10-methanol
DTXSID20235817



Benzo(a)pyrene-10-sulfonic acid, 7,8,9,10-tetrahydro-7,8,9-trihydroxy-, (7alpha,8beta,9beta)
DTXSID80154378



Benzo(a)pyrene-11,12-diol
DTXSID70215609



Benzo(a)pyrene-11,12-diol, 11,12-dihydro-, cis-
DTXSID20214501

- Type ahead search using Names, synonyms and CASRNs
- Millions of identifiers
- Substring search

Search Results

Searched with 'Synonym Substring': Benzo(A)Pyrene

183 chemicals

Search for classes of chemicals

- Examples: “perfluoro”

Chemicals

Product/Use Categories

Assay/Gene

perfluoro

☒ Identifier substring search

Search Results

Searched with 'Synonym Substring': Perfluoro

Select all



Download

Send to Batch Search

Substring



DTXSID

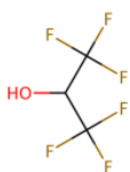
CASRN

TOXCAST

2098 chemicals

Hide chemicals that are:

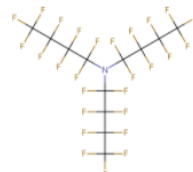
Filter by Name or CASRN



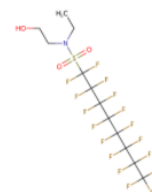
2H-Perfluoro-2-propanol
DTXSID:DTXSID1022134
CASRN:920-66-1
TOXCAST:-



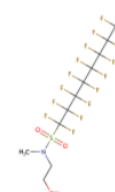
Perfluorooctanesulfonyl fluoride
DTXSID:DTXSID5027140
CASRN:307-35-7
TOXCAST:-



Perfluorotributylamine
DTXSID:DTXSID0027141
CASRN:311-89-7
TOXCAST:-



N-Ethyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide
DTXSID:DTXSID6027426
CASRN:1691-99-2
TOXCAST:-



N-Methyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide
DTXSID:DTXSID7027831
CASRN:24448-09-7
TOXCAST:-

0 related chemical
structures with this
substance

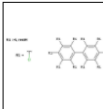
Perfluoro compounds, C5-18
DTXSID:DTXSID5029059
CASRN:86508-42-1
TOXCAST:7/235



Search for classes of chemicals

Examples:

- PCBs (or polychlorinated biphenyls)



Polychlorinated biphenyls

1336-36-3 | DTXSID5024267

Searched by DSSTox Substance Id.

Quality Control Notes

biphenyl with multiple (unknown number) chlorines attached at unknown locations

Intrinsic Properties

Presence in Lists

Federal





- National Recommended Water Quality Criteria Aquatic Life chemical list
- EPA Region 10
- EPA: Toxics Release Inventory
- EPA: Underground Storage Tanks (USTs)
- EPA: IRIS
- State-Specific Water Quality Standards Effective under the Clean Water Act (CWA)
- ENDOCRINE: EDSP21 Tier 1 Screening Chemicals: List 2
- ENDOCRINE: EDSP Universal Screening Chemicals: List 1



- Polycyclic aromatic hydrocarbons

Polycyclic aromatic hydrocarbons

130498-29-2 | DTXSID3044043

Searched by Expert Validated Synonym.

Select all Download Send to Batch Search Relationship     73 chemicals

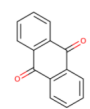
Hide chemicals that are:  Filter by Name or CASRN 

Searched Chemical


73 related chemical structures with this substance

Polycyclic aromatic hydrocarbons
DTXSID:DTXSID3044043
CASRN:130498-29-2
TOXCAST:-

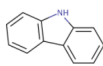
Component


Anthraquinone
DTXSID:DTXSID020095
CASRN:84-65-1
TOXCAST:235

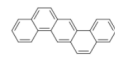
Component


Benzofluorene
DTXSID:DTXSID020139
CASRN:86-32-8
TOXCAST:72/235

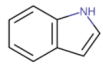
Component


Carbazole
DTXSID:DTXSID4020248
CASRN:86-74-8
TOXCAST:39/598

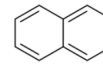
Component


Dibenz(a,h)anthracene
DTXSID:DTXSID9020409
CASRN:53-70-3
TOXCAST:61/621

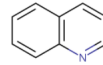
Component


Indole
DTXSID:DTXSID002737


Component


Naphthalene
DTXSID:DTXSID002813

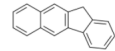
Component


Quinoline
DTXSID:DTXSID002138

Component


Chrysene
DTXSID:DTXSID002437

Component


2,3-Benzofluorene
DTXSID:DTXSID002477

QUESTION 1

- How many “conazoles” are in the dashboard?

29

56

125

321

Challenges with Nomenclature

- Be CAREFUL with names! There is a LOT of confusion in the public domain. CHOOSE sources wisely!
- There are MANY public databases but not many are curated
- All public databases have value but not many curate data
- Example: METHANE on PubChem
<https://pubchem.ncbi.nlm.nih.gov/compound/297>

CAS Registry Numbers on PubChem

2.3.1 CAS



74-82-8

- ▶ CAMEO Chemicals; CAS Common Chemistry; ChemIDplus; DrugBank; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECH...

8006-14-2

- ▶ CAMEO Chemicals; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECHA)

7440-44-0

- ▶ ChemIDplus

7782-40-3

- ▶ ChemIDplus

7782-42-5

- ▶ ChemIDplus

16291-96-6

- ▶ ChemIDplus

64365-11-3

CASRN lookup on the dashboard

Search Results

Searched using Batch Search

8 chemicals

Select all

Download

Send to Batch Search

Default



CASRN

DTXSID

Molecular Formula



Hide chemicals that are:

Filter by Name or CASRN



[Methane](#)

CASRN:74-82-8

DTXSID:DTXSID8025545

Molecular Formula:CH4



[Carbon](#)

CASRN:7440-44-0

DTXSID:DTXSID9027651

Molecular Formula:C

0 related chemical
structures with this
substance

[Natural gas](#)

CASRN:8006-14-2

DTXSID:DTXSID2027676

Molecular Formula:-

2 related chemical
structures with this
substance

[Graphite](#)

CASRN:7782-42-5

DTXSID:DTXSID2049634

Molecular Formula:-

1 related chemical
structure with this
substance

[Charcoal](#)

CASRN:16291-96-6

DTXSID:DTXSID2051217

Molecular Formula:-

1 related chemical
structure with this
substance

[Diamond](#)

CASRN:7782-40-3

DTXSID:DTXSID10905072

Molecular Formula:-

0 related chemical
structures with this
substance

[Activated charcoal](#)

CASRN:64365-11-3

DTXSID:DTXSID801019028

Molecular Formula:-

1 related chemical
structure with this
substance

[Carbon nanotubes](#)

CASRN:308068-56-6

DTXSID:DTXSID301020377

Molecular Formula:-

Methane is Diamond and Nanotubes?

- These are all Depositor Names for Methane ☹️

2.4.2 Depositor-Supplied Synonyms



UN 1971 (Salt/Mix)	Fullerene soot, (as produced)	Carbon Nanotube sponges XFCN01	DTXSID9027651
UN 1972 (Salt/Mix)	MWNTs Butyl acetate suspension	Carbon Nanotube sponges XFCN07	Graphite electrode, rotrode disc
Activated carbon, pellets 3mm	QuadraPure C, 0.3-0.8mm	Carbon Nanotube sponges XFCN08	Carbon conductive cement adhesive
Graphene quantum dots(Powder)	6GRV67N0U2	Carbon, activated, -4+8 mesh	Conductive Flexible TPU Filament
Multiwall Nanotubes 5-15 nm	GO quantum dots yellow(Powder)	Carbon, activated, 2mm & down	GO quantum dots yellow(1mg/ml)
GO quantum dots(C: 1mg/ml)	Graphene electric aqueous slurry	CHEMBL2106049	Graphite powder, -20+84 mesh
;) MWNTs ethyl acetate suspension	Graphene powder Physical methods	Diamond Synthesized, 95% Nano	Carbon black, Super P Conductive
Reduced Graphene Oxide@ SnO2	Reduced Graphene Oxide@ Co3O4	Diethyl Cyanomethyl Phosphonate	DTXSID50179391
Carbon nanotubes aqueous slurry	Carbon Conductive Adhesive Tapes	DTXSID8025545	NanoIntegris metallic SWCNTs70%



QUESTION 1

- How many “conazoles” are in the dashboard?

29

56

125

321

Detailed Chemical Pages

One more identifier – the **DTXSID**

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ SAFETY

▶ ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS


GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

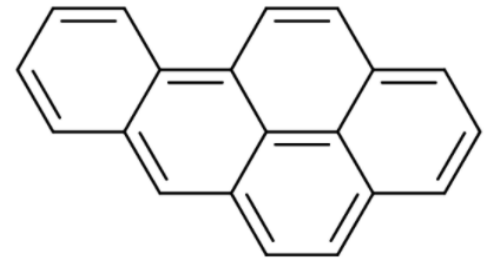
▶ LITERATURE

LINKS



Benzo(a)pyrene
50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.





Wikipedia


Benzo[a]pyrene is a polycyclic aromatic hydrocarbon and the result of incomplete combustion of organic matter at temperatures between 300 °C (572 °F) and 600 °C (1,112 °F). The ubiquitous compound can be found in coal tar, tobacco smoke and many foods, especially grilled meats. The substance with the formula C₂₀H₁₂ is one of the benzopyrenes, formed by a benzene ring fused to pyrene. Its diol epoxide metabolites (more commonly known as BPDE) react and bind to ...
[Read more](#)


Quality Control Notes


Intrinsic Properties


 Molecular Formula: C₂₀H₁₂

 Mol File

 Find All Chemicals

 Average Mass: 252.316 g/mol

 Isotope Mass Distribution

 Monoisotopic Mass: 252.0939 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

- Chemical page: Wikipedia snippet when available, intrinsic properties, structural identifiers, linked substances

DTXSID as a substance identifier

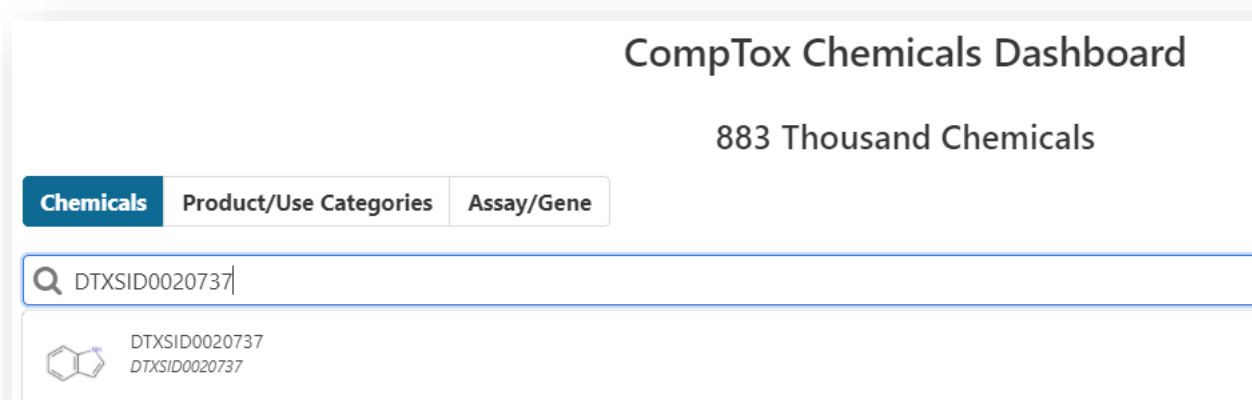
- Blessed now by Wikipedia
- In MANY public databases – ChemSpider, PubChem, eChemPortal
- Increasingly used across all EPA databases
- Easy to use/search



Property Discussion

DSSTox substance ID (P3117)


DSSTox substance identifier (DTXSID) used in the Environmental Protection Agency CompTox Dashboard
DTXSID | DTXSID ID



- URL linking: <https://comptox.epa.gov/dashboard/DTXSID0020737>
- ANY database can link directly via DTXSIDs...more later..

Detailed Chemical Pages

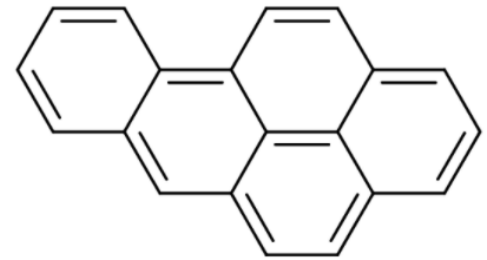
Easy Navigation



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.



DETAILS




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



Wikipedia


Benzo[a]pyrene is a polycyclic aromatic hydrocarbon and the result of incomplete combustion of organic matter at temperatures between 300 °C (572 °F) and 600 °C (1,112 °F). The ubiquitous compound can be found in coal tar, tobacco smoke and many foods, especially grilled meats. The substance with the formula C₂₀H₁₂ is one of the benzopyrenes, formed by a benzene ring fused to pyrene. Its diol epoxide metabolites (more commonly known as BPDE) react and bind to ...
[Read more](#)

Quality Control Notes

Intrinsic Properties

 **Molecular Formula:** C₂₀H₁₂  Mol File  Find All Chemicals

 **Average Mass:** 252.316 g/mol  Isotope Mass Distribution

 **Monoisotopic Mass:** 252.0939 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

- Chemical page: Wikipedia snippet when available, intrinsic properties, structural identifiers, linked substances

From the Chemical Details Page... all chemicals with same FORMULA

Intrinsic Properties



Molecular Formula: C₂₀H₁₂




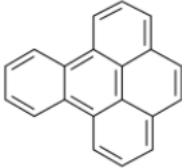
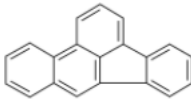
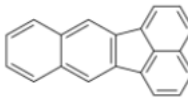
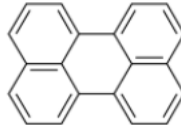
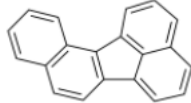
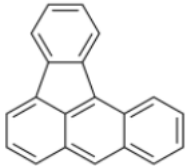
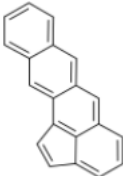
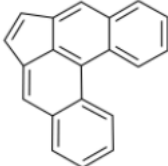
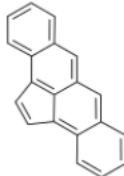
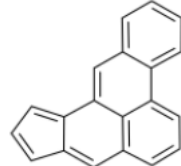
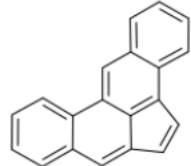
Mol File

 Find All Chemicals

Search Results

Searched by Exact Molecular Formula: C₂₀H₁₂.

Download ▾ Send to Batch Search Default ▾ CASRN X DTXSID X ▾ 27 chemicals Hide chemicals that are: ▾ Filter by Name or C

 <p>Benzo(a)pyrene CASRN:50-32-8 DTXSID:DTXSID2020139</p>	 <p>Benzo(e)pyrene CASRN:192-97-2 DTXSID:DTXSID3023764</p>	 <p>Benzo(b)fluoranthene CASRN:205-99-2 DTXSID:DTXSID0023907</p>	 <p>Benzo(k)fluoranthene CASRN:207-08-9 DTXSID:DTXSID0023909</p>	 <p>Perylene CASRN:198-55-0 DTXSID:DTXSID4047753</p>	 <p>Benzo(j)fluoranthene CASRN:205-82-3 DTXSID:DTXSID8052691</p>
 <p>Benzo[a]fluoranthene CASRN:203-33-8 DTXSID:DTXSID4059756</p>	 <p>Cyclopenta(de)naphthalene CASRN:16683-64-0 DTXSID:DTXSID80168197</p>	 <p>Benz(a)acephenanthrylene CASRN:192-28-9 DTXSID:DTXSID70172748</p>	 <p>Cyclopenta(fg)naphthalene CASRN:19770-52-6 DTXSID:DTXSID40173469</p>	 <p>Benzo(de)cyclopent(a)anthracene CASRN:198-46-9 DTXSID:DTXSID60173507</p>	 <p>Benz(e)aceanthrylene CASRN:199-54-2 DTXSID:DTXSID30173675</p>

How many chemicals are associated through LINKED SUBSTANCES?

- Atrazine, is a herbicide – in MANY commercial products
- The dashboard has salt forms, isotopically labelled forms, multicomponent forms
- How do we identify what they are???

Linked Substances

Same Connectivity: [6 records](#) (based on first layer of InChI)


Mixtures, Components and Isotopomers: [DTXCID90112: 25 records;](#)


Similar Compounds: [73 records](#) (based on Tanimoto coefficient >0.8)


A little more about the InChI


- An InChIKey is made up of two blocks...
 - Block 1 – “the connectivity” of atoms and bonds
 - Block 2 – isotopes, charge, stereo

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

 **InChI String:** InChI=1S/C8H14ClN5/c1-4-10-7-12-6(9)13-8(14-7)11-5(2)3/h5H,4H2,1-3H3,(H2,10,11,12,13,14)

 **InChIKey:** MXWJVTOOROXGIU-UHFFFAOYSA-N

Search Google for:

- The InChIKey is VERY USEFUL

- Demo an internet search using InChIs – Cholesterol has the InChIKey: HVYWMOMLDIMFJA-DPAQBDIFSA-N
- Demo Atrazine – Linked Substances – Skeleton
- More about Linked Substances....

Linked Substances – more interesting

- We map chemicals together using cheminformatics approaches
- Use desalting, destereo, split multicomponents etc to map chemicals together

McEachran et al. *J Cheminform* (2018) 10:45
<https://doi.org/10.1186/s13321-018-0299-2>

Journal of Cheminformatics

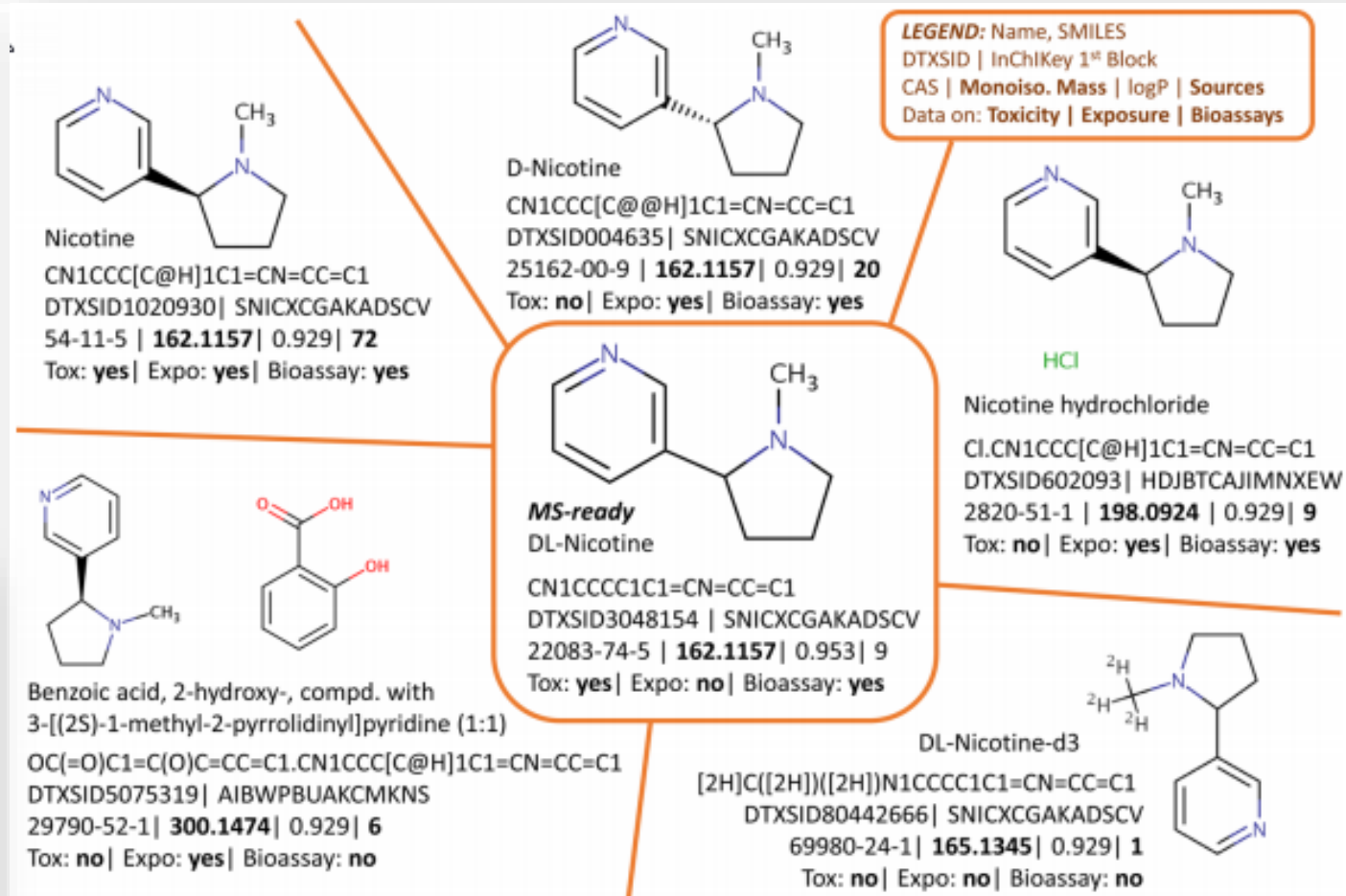
METHODOLOGY

Open Access



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

Andrew D. McEachran^{1,2*}, Kamel Mansouri^{1,2,3}, Chris Grulke², Emma L. Schymanski⁴, Christoph Ruttkies⁵ and Antony J. Williams^{2*}

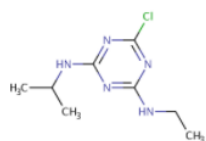


Atrazine Linked Substances

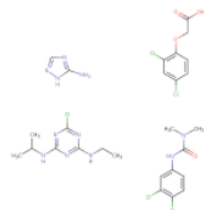
MS-Ready Mappings of Atrazine (Isotopes pre-filtered)

20 of 25 chemicals visible

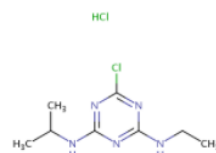
Select all Download Send to Batch Search Default DTXSID CASRN TOXCAST Isotopes Filter by Name or CASRN



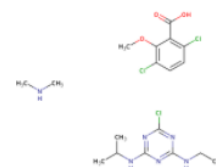
Atrazine
DTXSID:DTXSID9020112
CASRN:1912-24-9
TOXCAST:62/1024



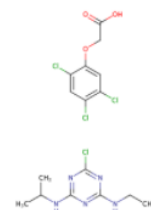
Anox M
DTXSID:DTXSID50156021
CASRN:128996-76-9
TOXCAST:-



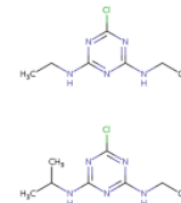
s-Triazine, 2-chloro-4-(ethylamino)-6-(isopropylamino)-1,3,5-triazine hydrochloride
DTXSID:DTXSID30165459
CASRN:15386-47-7
TOXCAST:-



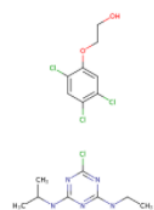
Marksman
DTXSID:DTXSID80166936
CASRN:160544-50-3
TOXCAST:-



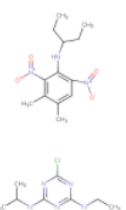
Acetic acid, (2,4,5-trichlorophenoxy)-, methyl ester
DTXSID:DTXSID70192527
CASRN:39283-62-0
TOXCAST:-



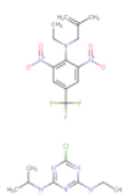
1,3,5-Triazine-2,4-diamine, 6-chloro-N,N-dimethyl-
DTXSID:DTXSID60192556
CASRN:39331-45-8
TOXCAST:-



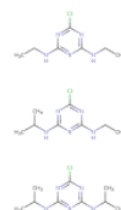
Buvinol
DTXSID:DTXSID10199555
CASRN:51602-05-2
TOXCAST:-



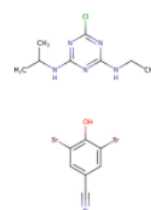
Atrazine mixture with pendimethalin
DTXSID:DTXSID10209527
CASRN:60704-01-0
TOXCAST:-



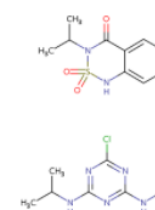
Maizor
DTXSID:DTXSID20215154
CASRN:64867-15-8
TOXCAST:-



Polytriazine
DTXSID:DTXSID00222508
CASRN:72172-70-4
TOXCAST:-



Benzonitrile, 3,5-dibromo-4-hydroxy-, methyl ester
DTXSID:DTXSID20226063
CASRN:75084-56-9
TOXCAST:-



Bentazon / atrazine
DTXSID:DTXSID80226064
CASRN:75084-57-0
TOXCAST:-

QUESTION 2

- How many salts of perfluorooctanesulfonic acid are there?

6

15

18

43

A little more about our data quality

- Five full time curators register and curate data to elevate quality

Record Information



Citation: U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. <https://comptox.epa.gov/dashboard/DTXSID0020022> (accessed October 18, 2020), 5-(2-Chloro-4-(trifluoromethyl)phenoxy)-2-nitrobenzoic 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

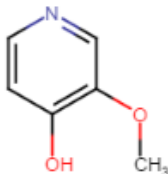
Underneath the Dashboard

View/Edit a Single Record Structure Search Browse/Curate Records Export DSSTox Chemotypes Manage Chemical Lists Manage Property Data Add Deleted Casms

Preferred Name matched null
You are viewing the record associated with
DTXSID80198757
CASRN: 62885-41-0

4-Hydroxy-3-methoxy

Valid license cannot be found



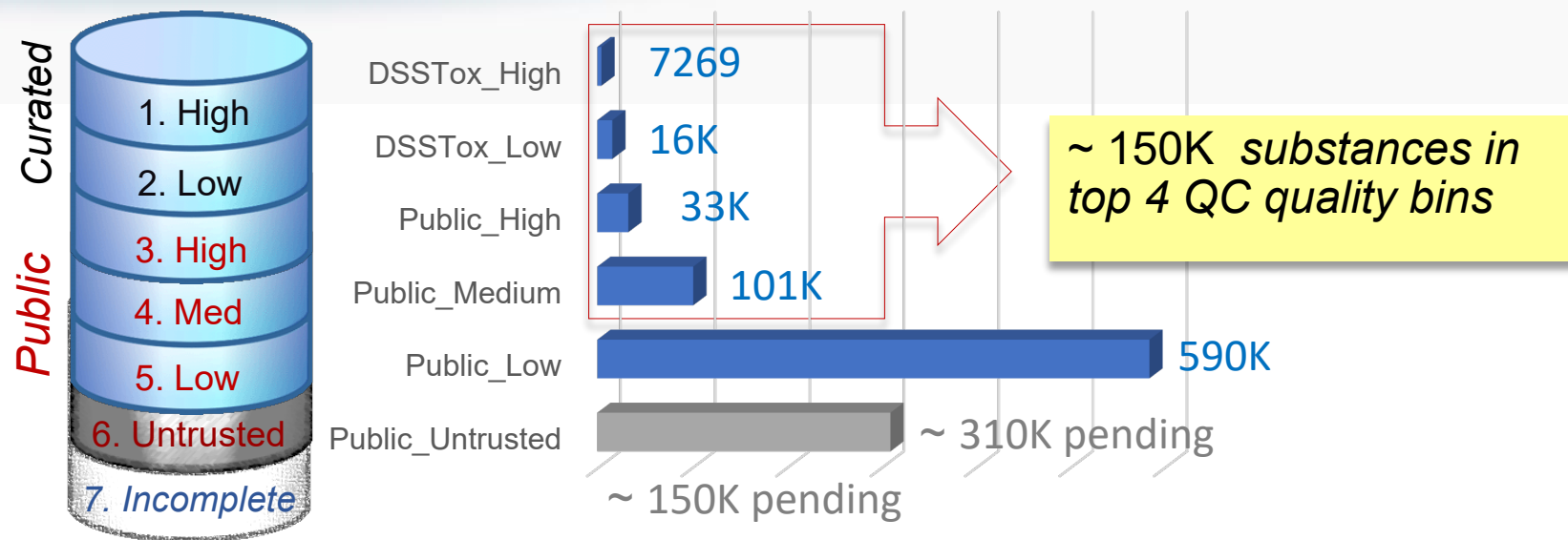
Chemical structure diagram of 4-Hydroxy-3-methoxypyridine, showing a pyridine ring with a hydroxyl group at position 4 and a methoxy group at position 3.

Calculate from Structure

Substance_ID:	DTXSID80198757	Compound_ID:	DTXCID40121248
CAS:	62885-41-0	Chemical Shown:	Tested Chemical
Name:	4-Hydroxy-3-methoxypyridine	Private Notes:	
Substance Type:	Single Compound	Source of CAS-Compound:	STN(DSSTox)
QC Level:	DSSTox_High	Double Stereo:	None
Data Source:	STN(DSSTox)	Chiral Stereo:	None
QC Notes:	CAS [50700-60-2] assigned by DSSTox to pyridin-one tautomer form, which resolves to hydroxy form thru InChI	Chemical Form:	Organic
		Organic Form:	Parent

Distribution of curated data

Now at >910k substances



QC Levels

DSSTox_High: Hand curated and validated

DSSTox_Low: Hand curated and confirmed using multiple public sources

Public_High: Extracted from EPA SRS and confirmed to have no conflicts in ChemID and PubChem

Public_Medium: Extracted from ChemID and confirmed to have no conflicts in PubChem

Public_Low: Extracted from ACToR or PubChem

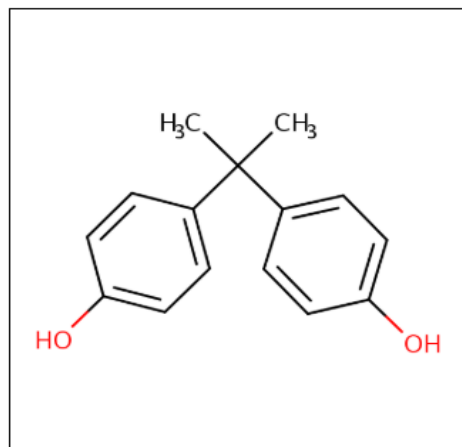
Public_Untrusted: Postulated, but found to have conflicts in public sources

Record Information Quality Flags

Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.



Wikipedia


Intrinsic Properties

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

 **Citation:** U.S. Environmental Protection Agency. Chemistry Dashboard. <https://comptox.epa.gov/dashboard/DTXSID7020182> (accessed Aug 20th, 2018), Bisphenol A

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

Record Information

 **Citation:** U.S. Environmental Protection Agency. Chemistry Dashboard. <https://comptox.epa.gov/dashboard/DTXSID7020182> (accessed Aug 20th, 2018), Bisphenol A

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

ChemReg Curation

The ALANWOOD Pesticide Set

View/Edit a Single Record Structure Search Browse/Curate Records Export DSSTox Chemotypes **Manage Chemical Lists** Manage Property Data Add Deleted Casms Welcome, Chris Logout

Welcome cgrulke

Editing Listname: ALANWOOD

External Check Results	
Description	Records
Curator Validated	1216
Resolved Duplicates	0
Ignored	0
Structure matched STRUCTURE Preferred Name matched NAME CAS-RN matched CASRN	2
Structure matched STRUCTURE Valid Synonym matched NAME CAS-RN matched CASRN	71
Structure matched STRUCTURE Unique Synonym matched NAME CAS-RN matched CASRN	106
Structure matched STRUCTURE Unique Synonym matched NAME Other CAS-RN matched CASRN	2
Structure matched	

Substance Mapping						
(1 of 5) 1 2 3 4 5 25 ▾						
	Source Casrn	Source Name	Hit Substance_ID	Hit Casrn	Hit Name	
1	88-82-4	2,3,5-tri-iodobenzoic acid	DTXSID4041317	88-82-4	2,3,5-Triiodobenzoic acid	Validate Mapping
2	50-31-7	2,3,6-TBA	DTXSID6040296	50-31-7	2,3,6-Trichlorobenzoic acid	Validate Mapping
3	122-88-3	4-CPA	DTXSID9034282	122-88-3	4-Chlorophenoxyacetic acid	Validate Mapping
4	126448-41-7	acibenzolar	DTXSID20155187	126448-41-7	Acibenzolar [ISO]	Validate Mapping
5	76636-10-7	amibuzin	DTXSID20227459	76636-10-7	Amibuzin [ISO]	Validate Mapping
6	3566-10-7	amobam	DTXSID0058067	3566-10-7	Ambam	Validate Mapping
7	86-88-4	antu	DTXSID8020919	86-88-4	1-(1-Naphthyl)-2-thiourea	Validate Mapping
8	52-46-0	apholate	DTXSID7073149	52-46-0	1,3,5,2,4,6-Triazatriphosphorine, 2,2,4,4,6,6-hexakis(1-aziridinyl)-2,2,4,4,6,6-hexahydro-	Validate Mapping
9	3586-60-5	asomate	DTXSID70189412	3586-60-5	Arsine, tris(dimethyldithiocarbamoyl)	Validate Mapping
10	28956-64-1	bentaluron	DTXSID30183153	28956-64-1	Bentaluron [ISO]	Validate Mapping
11	21564-17-0	benthiazole	DTXSID6032647	21564-17-0	2-(Thiocyanomethylthio)benzoic acid	Validate Mapping
12	1022-46-4	bentranil	DTXSID60144732	1022-46-4	4H-3,1-Benzoxazin-4-one, 2-phenyl-	Validate Mapping

A little more about our data quality

Computational Toxicology 12 (2019) 100096



ELSEVIER

Contents lists available at [ScienceDirect](#)

Computational Toxicology

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

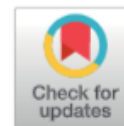


EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research

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

^a National Center for Computational Toxicology, Office of Research & Development, US Environmental Protection Agency, Mail Drop D143-02, Research Triangle Park, NC 27711, USA

^b Senior Environmental Employment Program, US Environmental Protection Agency, Research Triangle Park, NC 27711, USA



QUESTION 2

- How many salts of perfluorooctanesulfonic acid are there?

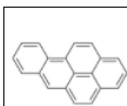
6

15

18

43

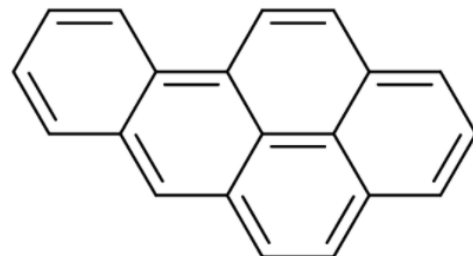
Navigating data via the Left Hand Tabs



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.



DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ SAFETY

▶ ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

▶ LITERATURE

LINKS

Wikipedia

Benzo[a]pyrene is a polycyclic aromatic hydrocarbon and the result of incomplete combustion of organic matter at temperatures between 300 °C (572 °F) and 600 °C (1,112 °F). The ubiquitous compound can be found in coal tar, tobacco smoke and many foods, especially grilled meats. The substance with the formula $C_{20}H_{12}$ is one of the benzopyrenes, formed by a benzene ring fused to pyrene. Its diol epoxide metabolites (more commonly known as BPDE) react and bind to

...
[Read more](#)

Quality Control Notes

Intrinsic Properties



Molecular Formula: $C_{20}H_{12}$



Mol File



Find All Chemicals



Average Mass: 252.316 g/mol



Isotope Mass Distribution



Monoisotopic Mass: 252.0939 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

“Executive Summary”

Executive Summary

Quantitative Risk Assessment Values

- ✓ IRIS values available [↗](#)
- ✗ No PPRTV values
- ✓ EPA RSL values available [↗](#)
- ✓ Minimum RfD: **0.00030 mg/kg-day** (chronic, IRIS, oral, 8) [↗](#)
- ✓ Minimum RfC: **0.0000020 mg/m3** (chronic, IRIS, inhalation, 8) [↗](#)
- ✗ IVIVE POD not calculated

Quantitative Hazard Values

- ✓ Minimum oral POD: **0.070 mg/kg-day** (chronic, EFSA, oral, 5) [↗](#)
- ✓ Minimum inhalation POD: **0.0046 mg/m3** (chronic, IRIS, inhalation, 8) [↗](#)
- ✓ Lowest Observed Bioactivity Equivalent Level: [AR](#)

Cancer Information

- ✓ Cancer slope factor: **23.5 (mg/kg-day)-1** (ACToR, dermal, 4) [↗](#)
- ✓ Inhalation unit risk: **2.4 (mg/m3)-1** (IRIS, inhalation, 8) [↗](#)
- ✓ Carcinogenicity data available: IARC: undefinedEPA OPP cancer class: undefinedNTP Report on Carcinogens (ROC 12): undefinedNLM ToxNet HSDB carcinogenicity warningUniversity of Maryland carcinogenicity warning, [↗](#)
- ✗ No genotoxicity findings reported

Reproductive Toxicology

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

Chronic Toxicology

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

Subchronic Toxicology

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

Developmental Toxicology

- ✗ No developmental toxicity data available.

Acute Toxicology

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

Subacute Toxicology

- ✗ No subacute toxicity data available.

Neurotoxicology

- ✗ No neurotoxicology data available.

Endocrine System

- ✓ Endocrine Disruption Potential: Significant Estrogen Receptor activity seen. Chemical was positive in **7 ER assays** (out of 12) and was positive in **3 AR assays** (tested in 6).

ADME

- ✗ No HTTK data

Fate and Transport

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

Exposure

- ✓ Exposure Estimates have been predicted using the SEEM modeling methodology [↗](#)

AOP Information

- ✓ AOP Links: [36](#), [61](#), [66](#), [107](#), [150](#), [163](#), [187](#), [200](#)

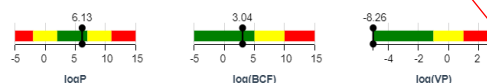
Other Notes

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

REGIONAL SCREENING

Class	THQ	Value
GIABS (-)	THQ = 0.1	1
ABS (-)	THQ = 0.1	0.13
MCL (ug/L)	THQ = 0.1	0.2
MCLbased SSL (mg/kg)	THQ = 0.1	0.24
cancer slope factor ((mg/kg-day)-1)	THQ = 0.1	1
cancer unit risk ((ug/m3)-1)	THQ = 0.1	0.0006
RfDo (mg/kg-day)	THQ = 0.1	0.0003
RfCi (mg/m3)	THQ = 0.1	0.000002
Resident soil (mg/kg)	THQ = 0.1	0.11
Industrial soil (mg/kg)	THQ = 0.1	2.1
Resident air (ug/m3)	THQ = 0.1	0.00021
Industrial air (ug/m3)	THQ = 0.1	0.00088
Tapwater (ug/L)	THQ = 0.1	0.025
Riskbased SSL (mg/kg)	THQ = 0.1	0.029
GIABS (-)	THQ = 1	1
ABS (-)	THQ = 1	0.13
MCL (ug/L)	THQ = 1	0.2
MCLbased SSL (mg/kg)	THQ = 1	0.24
cancer slope factor ((mg/kg-day)-1)	THQ = 1	1
cancer unit risk ((ug/m3)-1)	THQ = 1	0.0006
RfDo (mg/kg-day)	THQ = 1	0.0003
RfCi (mg/m3)	THQ = 1	0.000002
Resident soil (mg/kg)	THQ = 1	0.11
Industrial soil (mg/kg)	THQ = 1	2.1
Resident air (ug/m3)	THQ = 1	0.0017
Industrial air (ug/m3)	THQ = 1	0.0088
Tapwater (ug/L)	THQ = 1	0.025
Riskbased SSL (mg/kg)	THQ = 1	0.029

PHYSICHEM PARAMETERS



- Overview of toxicity-related info
 - Quantitative values
 - Info re. toxicology subsets
 - Physchem. and Fate & Transport
 - Adverse Outcome Pathway links
 - *In vitro* bioactivity summary plot


Quantitative Risk Assessment Values

- ✓ IRIS values available [↗](#)
- ✗ No PPRTV values
- ✓ EPA RSL values available [↗](#)
- ✓ Minimum RfD: **0.00030 mg/kg-day** (chronic, IRIS, oral, 8) [↗](#)
- ✓ Minimum RfC: **0.0000020 mg/m3** (chronic, IRIS, inhalation, 8) [↗](#)
- ✗ IVIVE POD not calculated

Quantitative Hazard Values

- ✓ Minimum oral POD: **0.070 mg/kg-day** (chronic, EFSA, oral, 5) [↗](#)
- ✓ Minimum inhalation POD: **0.0046 mg/m3** (chronic, IRIS, inhalation, 8) [↗](#)
- ✓ Lowest Observed Bioactivity Equivalent Level: [AR](#)

Experimental and Predicted Data



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Property

Summary

Download Columns

Property	Experimental average	Predicted average
Water Solubility	8.40e-9 (4)	1.75
LogKow: Octanol-Water	6.13 (2)	6.24
Vapor Pressure	5.49e-9 (1)	3.61e-9
Boiling Point	495 (3)	480
Henry's Law	4.57e-7 (1)	4.59e-7
Melting Point	177 (8)	189
Surface Tension	-	53.9
Flash Point	-	234
Density	-	1.28

- Physchem and Fate & Transport experimental and predicted data
- Data can be downloaded as Excel, TSV and CSV files
- Predictions: multiple algorithms
 - EPI Suite: Estimation Program Interface
 - ACD/Labs (commercial)
 - TEST: Toxicity Estimation Software Tool
 - OPERA: **O**PEn structure–activity/property **R**elationship **A**pp

ToxVal Database

- >50k chemicals
- >770k tox. values
- >30 sources of data
- ~5k journals cited
- ~70k citations

Hazard

DataType
Toxicity Value

Human Eco

Download Columns 10 Search query

More	Priority	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	7	cancer slope factor	-	chronic	23.5	(mg/kg-day)-1	-	dermal	-	Alaska DEC	Alaska DEC
	7	cancer unit risk	-	chronic	0.21	(mg/l)-1	-	inhalation	-	Alaska DEC	Alaska DEC
	7	cancer slope factor	-	chronic	3.08	(mg/kg-day)-1	-	inhalation	-	Alaska DEC	Alaska DEC
	7	cancer unit risk	-	chronic	0.88	(mg/m3)-1	-	inhalation	-	Alaska DEC	Alaska DEC
	7	cancer slope factor	-	chronic	7.3	(mg/kg-day)-1	-	oral	-	Alaska DEC	Alaska DEC
	7	MEG	Short-term Critical Air	short-term	80	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Marginal Air	short-term	15	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Soil Negligible Soil	chronic	12	mg/kg	-	Soil	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Long-Term, SL/d Negligible Water	chronic	0.0134	mg/L	-	oral	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Negligible Air	short-term	0.6	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD

<< < 1 2 3 4 > >>

Showing 1 to 10 of 32 records

[anced_search/index](#)

Let's talk about Export Formats

- Anywhere you see a table you can export
 - CSV is great for integration with other applications (plus read into Excel)
 - Excel file is generally the best for “viewing” as it can have multiple worksheets, color flagging of cells and offers all
- If you have cheminformatics tools SDF files are the best – view structures directly as concatenated “molfiles”
- Some examples... download file(s)

Advantages of Open Data

- By doing data exchange between databases you get to use other peoples work
- Linkages between systems (more later)
- Calling “APIs and Web Services” on the fly....
- SHOW EXAMPLES

GHS Data

Print Page

PUBCHEM > BENZO[A]PYRENE > LABORATORY CHEMICAL SAFETY SUMMARY (LCSS) > GHS CLASSIFICATION




CID 2336

Benzo[a]pyrene

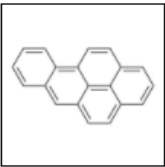
GHS Classification



Showing 6 of 6

Pictogram(s)	<div></div> <div>Irritant Health Hazard Environmental Hazard</div>
Signal	<u>Danger</u>
GHS Hazard Statements	H317: May cause an allergic skin reaction [<u>Warning</u> Sensitization, Skin] H340: May cause genetic defects [<u>Danger</u> Germ cell mutagenicity] H350: May cause cancer [<u>Danger</u> Carcinogenicity] H360FD: May damage fertility; May damage the unborn child [<u>Danger</u> Reproductive toxicity] H400: Very toxic to aquatic life [<u>Warning</u> Hazardous to the aquatic environment, acute hazard] H410: Very toxic to aquatic life with long lasting effects [<u>Warning</u> Hazardous to the aquatic environment, long-term hazard]
Precautionary Statement Codes	P201, P202, P261, P272, P273, P280, P281, P302+P352, P308+P313, P321, P333+P313, P363, P391, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)

Identifiers Support Searches in other systems



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Synonyms

Download

25

Search query

Synonym	Quality
Benzo(a)pyrene	Valid
Benzo[pqr]tetraphene	Valid
Benzo[a]pyrene	Valid
50-32-8 Active CAS-RN	Valid
BaP	Valid
Benzo[a]pyrene	Good
3,4-Benz[a]pyrene	Good
3,4-Benzopyrene	Good
3,4-Benzpyrene	Good
6,7-Benzopyrene	Good
BENZ(A)PYREN	Good
Benz(a)pyrene	Good
Benz[a]pyrene	Good

QUESTION 3

- How many CAS Registry Numbers does Atrazine have?

3

5

7

12

- CASRNs are very useful, and still limited
- Not every chemical has a STRUCTURE...substances vs structures
- “Chemical Abstracts Service” – numbers don’t exist until they abstracted and indexed
- Not every chemical on the dashboard necessarily has a CASRN – how would you find those that didn’t??? Hint: Search NOCAS_
- There are ~6000 chemicals without CASRN on the dashboard
- A chemical can also have many deleted CASRNs
- Where do you look for all identifiers for a chemical???

QUESTION 3

- How many CAS Registry Numbers does Atrazine have?

3

5

7

12

What chemicals are in hair care products?

Chemicals

Product/Use Categories

Assay/Gene

Q

hair

CPDat PRODUCT category: hair coloring
general hair coloring products which can not be classified into a more refined category

CPDat PRODUCT category: hair coloring hair bleach
products for lightening or removing color from hair on the head

CPDat PRODUCT category: hair coloring hair color - permanent
hair colors and dyes characterized as permanent

CPDat PRODUCT category: hair coloring hair color - professional
hair colors and dyes characterized as for professional use

CPDat PRODUCT category: hair coloring hair color activator
chemical activators for hair coloring products

CPDat PRODUCT category: hair coloring hair color developer
chemical developers for hair coloring products

CPDat PRODUCT category: hair styling and care dry shampoo
products for removing oil and dirt from hair

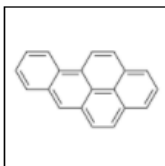
CPDat PRODUCT category: hair styling and care
general hair styling or hair care products which do not fit into a more refined category

Let's Talk Exposure



- Types of Exposure Data on the Dashboard
 - Consumer product categories and uses
 - Products containing the chemical
 - Predicted exposure levels from modeling (more in next session)

Sources of Exposure to Chemicals



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Chemical Weight Fractions

 Download ▾

Columns ▾

10 ▾

Search query

Product Name	Product Use Category	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source
m-525-1-5x pah mixtures 0.5 mg/ml for method 525	Not Yet Categorized:			MSDS	SIRI
mm6125 surface conditioner	Not Yet Categorized:			Health Product Declaration	Health Product Declaration Collaborative
monolithic membrane 6125 (mm6125) / monolithic membrane	Not Yet Categorized:			Health Product Declaration	Health Product Declaration Collaborative
organic potablewatr pw 32_component h:reg semi-volatile 690	Not Yet Categorized:	0.00	1.00e-3	MSDS	SIRI
polynuclear aromatic hydrocarbon mixture_ep84627	Not Yet Categorized:			MSDS	SIRI
prestone(r) power steering fluid	engine maintenance: auto fluids and additives			MSDS	CPCPdb
r-12 shield tite wet surface coating	Not Yet Categorized:	0.00	0.500	MSDS	SIRI
sea tar 1010_0028	Not Yet Categorized:			MSDS	SIRI
supelpreme-hc kit pah mix_48909	Not Yet Categorized:			MSDS	SIRI
supelpreme-hc pah mix 1ml_48905	Not Yet Categorized:			MSDS	SIRI

QUESTION 4

- How many consumer products are listed as containing chlorothalonil?

45 67 138 203

- Not every chemical has associated categories and uses
- MODELING data depends on QSAR predictions (structures)
- Data gathering continues unabated and has interesting sources

QUESTION 4

- How many consumer products are listed as containing chlorothalonil?

45

67

138

203

While we are discussing QSAR modeling

- What do you trust more? Experimental or predicted data?
 - Do you trust individual models or consensus models
 - What if there are no experimental data, how good are predictions?
-
- This will be covered a *little* in my next presentation and in way more detail in a later session

QUESTION 5

- What is the LogKow for fluconazole?

~0.2 ~0.3 ~0.5 ~3.4

How do we gather data for models

- We are continuously gathering data...where from?
 - How do we validate?
 - What can we check?
- Projects underway at present that may be of interest
 - Water Solubility dataset
 - Mass Spec Amenability
 - Eye and Skin Sensitization and Irritation
 - PFAS chemicals

QUESTION 5

- What is the LogKow for fluconazole?

~0.2

~0.3

~0.5

~3.4

QUESTION 6

- What is the brand name for Ketoconazole? (There may be more than one)

Glyphosate

Bisphenol A

Cialis

Nizoral

What's the best way to search the internet for chemical data?

- We know how complex chemicals identifiers are...
 - CASRN(s)
 - Hundreds of names (maybe)
 - SMILES
 - InChIs
 - EINECS, EC numbers
- What can WE do to help you navigate the internet?

QUESTION 6

- What is the brand name for Ketoconazole? (There may be more than one)

Glyphosate

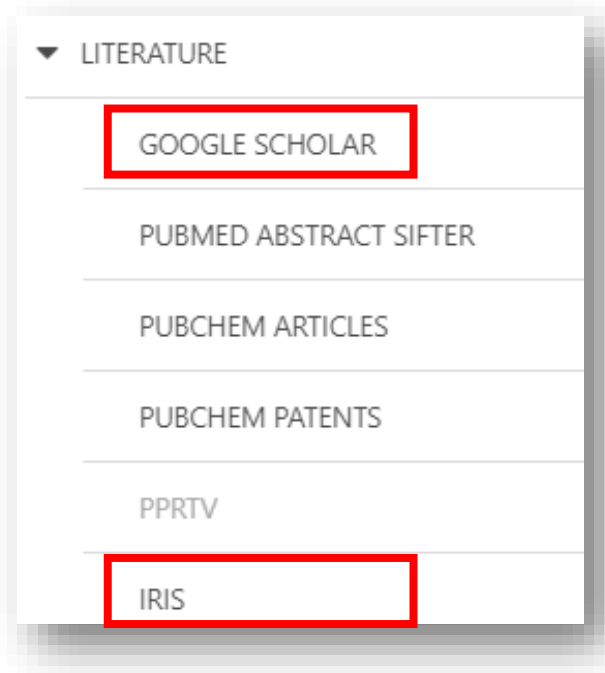
Bisphenol A

Cialis

Nizoral

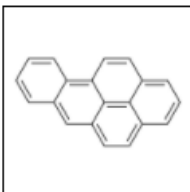
Identifiers are used in the app

- Identifiers are used to feed and link into “Literature”



A screenshot of the IRIS (Integrated Risk Information System) website for Benzo[a]pyrene (BaP). The page features the EPA logo and navigation links: Environmental Topics, Laws & Regulations, and About EPA. A search bar is present with the text 'Search EPA.gov'. The main heading is 'IRIS', followed by 'Benzo[a]pyrene (BaP)' and 'CASRN 50-32-8 | DTXSID2020139'. A list of links includes 'Toxicological Review (PDF)', 'IRIS Executive Summary (PDF)', and 'Supplemental Information on the IRIS Toxicological Review of Benzo[a]pyrene'. A table titled 'Noncancer Assessment' is displayed, showing the 'Reference Dose for Oral Exposure (RfD) (PDF)' and 'Last Updated: 01/19/2017'. The table has columns for System, RfD (mg/kg-day), Basis, and PoD. A 'Related Links' sidebar on the right contains a link to 'EPA Chemicals Dashboard - Benzo[a]pyrene (BaP)'. The left sidebar lists IRIS resources: IRIS Home, About IRIS, IRIS Recent Additions, IRIS Calendar, IRIS Assessments (highlighted), Advanced Search, IRIS Program Materials, and Contact Us.

System	RfD (mg/kg-day)	Basis	PoD




Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Abstract Sifter

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

Hazard 

Select a Query Term

Hazard

Fate and Transport

Metabolism/PK/PD

Chemical Properties

Exposure

Mixtures

Male Reproduction

Androgen Disruption

Female Reproduction

GeneTox

Cancer

Clinical Trials

Embryo and embryonic development

Child (infant through adolescent)

Dust and Exposure

Food and Exposure

Water and Exposure

Algae

Disaster / Emergency

Retrieve Articles 


Optionally, edit the query before retrieving.

("50-32-8" OR "Benzo(a)pyrene") AND (NOAEL OR NOEL OR LOEL OR Rfd OR "reference dose" OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])



- Real-time retrieval of data from PubMed (~30 million abstracts and growing)
- Choose from set of pre-defined queries
- Adjust and fine tune queries based on interests

Literature Searching

- “Sifting” of results using multiple terms
- Frequency counting terms
- Color highlighting of terms
- Download list to Excel
- Send list to PubMed for downloading ref. file
- Direct link via PubMed ID

To find articles quickly, enter terms to sift abstracts. 

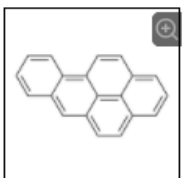
dermal cancer pyrene

<input type="checkbox"/>	dermal	cancer ↓	pyrene	Total	PMID	Year	Title	Authors	Journal	Rev
<input type="checkbox"/>	0	7	1	8	23922326	2013	Using immunotoxicity information to improve cancer risk a...	Zaccaria, McClure	International journal of toxicology	✓
<input type="checkbox"/>	8	7	2	17	16632147	2006	Development of a dermal cancer slope factor for benzo[a]...	Knafila, Philipps, Brecher, Petrovic, Richardson	Regulatory toxicology and pharmacology : RTP	✓
<input type="checkbox"/>	4	6	2	12	33359623	2020	Testing the validity of a proposed dermal cancer slope fac...	Magee; Forsberg	Regulatory toxicology and pharmacology : RTP	✓
<input type="checkbox"/>	0	5	1	6	28477805	2017	Pollution characteristics, sources and lung cancer risk of ...	Wang; Xia; Wu; Zhang; Sun; Yin; Zhou; Yang	Journal of environmental sciences (China)	
<input type="checkbox"/>	4	4	2	10	20888881	2010	Development and application of a skin cancer slope factor...	Knafila; Petrovic; Richardson; Campbell; Rowat	Regulatory toxicology and pharmacology : RTP	
<input type="checkbox"/>	4	4	1	9	16307791	2005	Health risk assessment on human exposed to environme...	Chen; Liao	The Science of the total environment	
<input type="checkbox"/>	2	4	1	7	11807932	2002	Cancer risk assessment for oral exposure to PAH mixtures.	Schneider; Roller, Kalberlah; Schuhmacher-Wolz	Journal of applied toxicology : JAT	
<input type="checkbox"/>	2	3	1	6	32460055	2020	PAHs in Chinese atmosphere Part II: Health risk assessm...	Ma; Zhu; Liu; Jia; Yang; Li	Ecotoxicology and environmental safety	
<input type="checkbox"/>	0	3	1	4	23379661	2013	Parent and halogenated polycyclic aromatic hydrocarbon...	Ni; Guo	Journal of agricultural and food chemistry	
<input type="checkbox"/>	0	3	1	4	20800879	2010	Health risk assessment on dietary exposure to polycyclic ...	Xia; Duan; Qiu; Liu; Wang; Tao; Jiang; Lu; Song; Hu	The Science of the total environment	
<input type="checkbox"/>	2	3	1	6	16293284	2005	Probabilistic risk assessment for personal exposure to car...	Liao; Chiang	Chemosphere	
<input type="checkbox"/>	0	2	1	3	17544483	2007	Health risk assessment for traffic policemen exposed to p...	Hu; Bai; Zhang; Wang; Zhang; Yu; Zhu	The Science of the total environment	
<input type="checkbox"/>	0	1	1	2	28795279	2017	Human health risk assessment and PAHs in a stretch of ri...	Srivastava; Sreekrishnan; Nema	Environmental monitoring and assessment	
<input type="checkbox"/>	0	1	1	2	12634119	2003	Deviation from additivity in mixture toxicity: relevance of n...	Lutz; Vamvakas; Kopp-Schneider; Schlatter; Stopper	Environmental health perspectives	
<input type="checkbox"/>	0	1	2	3	3709501	1986	The adsorption of polyaromatic hydrocarbons on natural a...	Menard; Noel; Khorami; Jouve; Dunnigan	Environmental research	
<input type="checkbox"/>	0	0	1	1	33136306	2020	Effects on Anical Outcomes of Regulatory Relevance of F...	Crumo; Boulanger; Farhat; Williams; Basu; Hecker	Environmental toxicology and chemistry	

Development of a dermal cancer slope factor for benzo[a]pyrene.
Polycyclic aromatic hydrocarbons (PAHs) are commonly found at environmentally impacted sites in both Canada and the United States, and also occur naturally. Typically, benzo[a]pyrene (B[a]P) is selected as a standard to which the cancer potencies of other carcinogenic PAHs are compared. Cancer potency estimates for B[a]P have been published for the oral and inhalation routes of exposure, however, no such estimate has been established by a regulatory agency for dermal exposure. The main objectives of the current investigation were to: evaluate approaches used to examine the relative carcinogenicity of PAHs; to conduct a review of mammalian dermal carcinogenicity studies for B[a]P; and derive a cancer slope factor for dermal exposure to PAHs using B[a]P as a surrogate for other PAHs. The toxicological database of dermal B[a]P studies was examined for relevant animal bioassays. Seven relevant studies were identified. A cancer slope factor for B[a]P was developed using the benchmark dose approach and the linearized multistage model. The upper 95th CI at the 5% effect level above background incidence was used as the point of departure for low-dose linear extrapolation. An average slope factor of 0.55 (microg/animal day)⁻¹ was calculated for mice, which was converted to a dose-equivalent slope factor of 25 (mg/kg day)⁻¹. This latter slope factor is proposed for application to human health risk assessment with no scaling adjustment. Dermal potency equivalency factor values were identified which may be used with other carcinogenic PAH in the calculation of total B[a]P equivalent dermal cancer risk estimates. An identified area for further investigation is the consideration of scaling in extrapolating the calculated dermal cancer slope factor from mice to humans.

External Links – Also use Identifiers Names, CASRN, PubChem IDs, InChIs...























Benzo(a)pyrene




















50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.




















General

-  EPA Substance Registry Service
-  PubChem
-  ChempSpider
-  CPCat
-  DrugBank
-  Wikipedia
-  MSDS Lookup
-  ChEMBL
-  ToxPlanet
-  ACS Reagent Chemicals
-  Wolfram Alpha
-  ECHA Infocard
-  ChemAgora
-  Consumer Product Information Database
-  ChEBI
-  NIST Chemistry Webbook
-  WEBWISER
-  PubChem Safety Sheet
-  Consumer Product Information Database
-  PubChem: Chemical Vendors













Toxicology

-  ACToR
-  DrugPortal
-  CCRIS
-  ChemView
-  CTD
-  eChemPortal
-  Gene-Tox
-  HSDB
-  ACToR PDF Report
-  CREST
-  National Air Toxics Assessment
-  ECOTOX
-  ChemView
-  Chemical Checker
-  BindingDB
-  CalEPA OEHHHA
-  NIOSH IDLH Values
-  LactMed
-  ECOTOX






Publications

-  Toxline
-  PPRTVWEB
-  PubMed
-  IRIS Assessments
-  EPA HERO
-  NIOSH Skin Notation Profiles
-  NIOSH Pocket Guide
-  RSC Publications
-  BioCaddie DataMed
-  Springer Materials
-  Bielefeld Academic Search Engine
-  CORE Literature Search
-  Google Books (Text Search)
-  Google Patents (Text search)
-  Google Scholar (Text search)
-  Google Patents (Structure search)
-  Google Books (Structure Search)
-  Google Scholar (Structure search)
-  Federal Register

Analytical

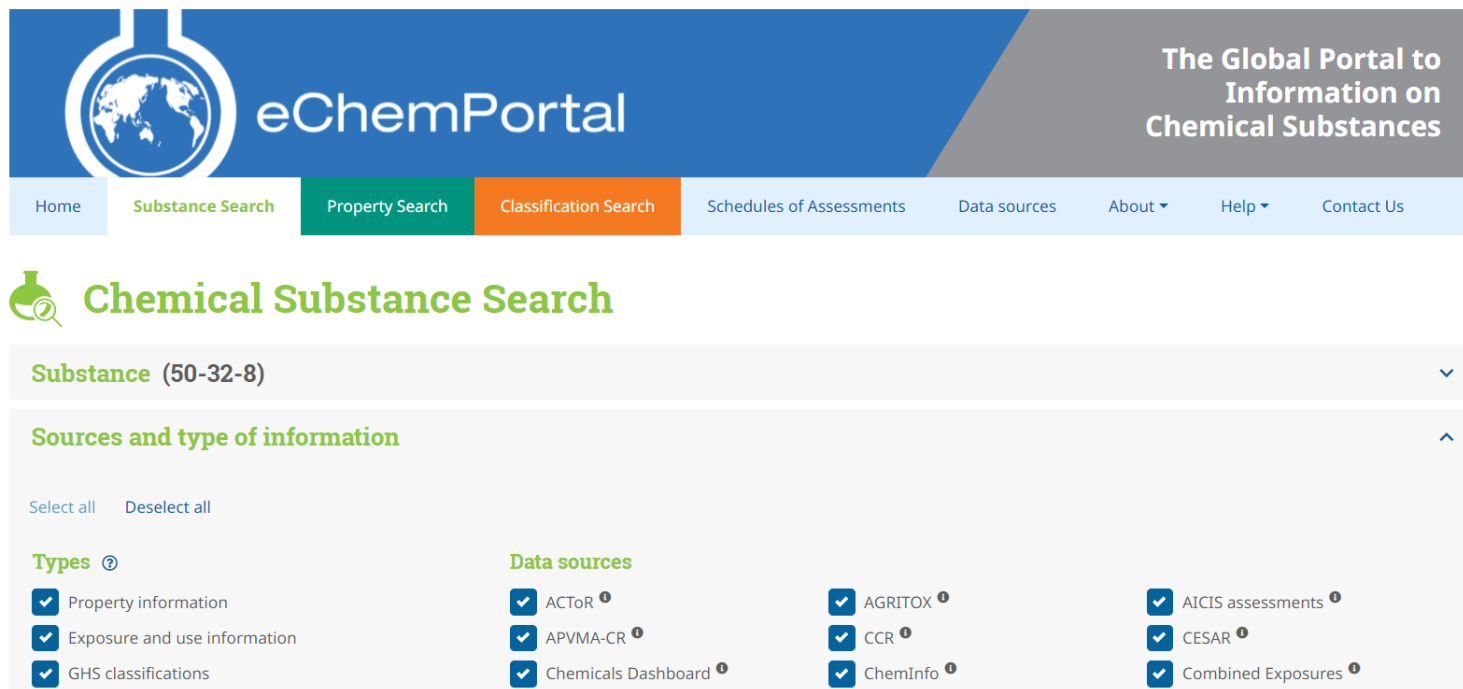
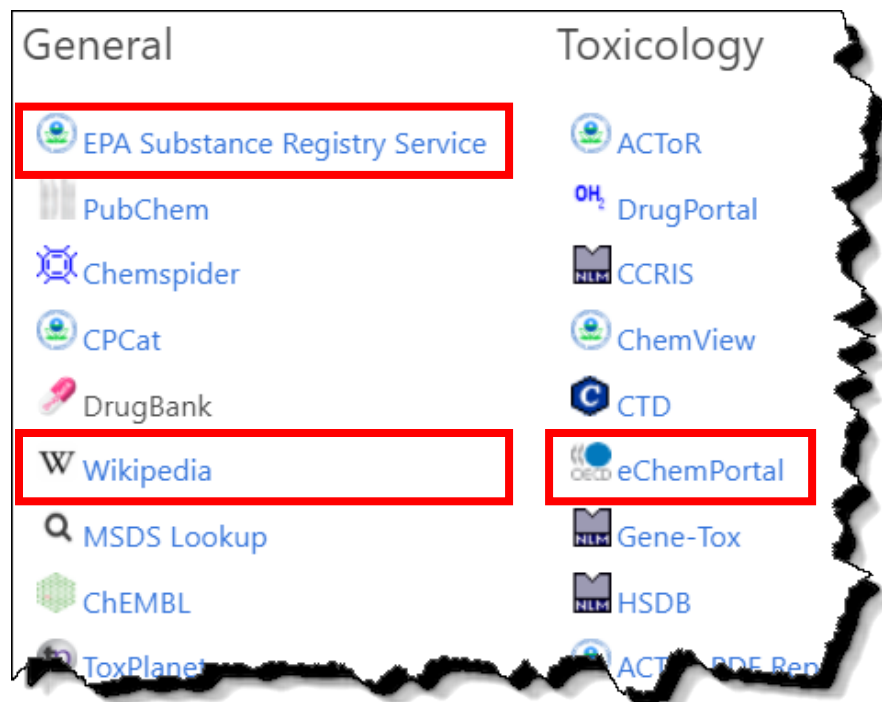
-  RSC Analytical Abstracts
-  Tox21 Analytical Data
-  MONA: MassBank North America
-  mzCloud
-  NIST IR Spectrum
-  NIST MS Spectrum
-  MassBank
-  NIST Antoine Constants
-  IR Spectra on PubChem
-  NIST Kovats Index values
-  Protein DataBank
-  National Environmental Methods Index

Prediction

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

External Links

- Links to ~90 websites providing access to additional data on the chemical of interest



The screenshot shows the eChemPortal website. The header features the OECD logo and the text 'The Global Portal to Information on Chemical Substances'. Below the header is a navigation bar with links: Home, Substance Search (highlighted), Property Search, Classification Search, Schedules of Assessments, Data sources, About, Help, and Contact Us. The main content area is titled 'Chemical Substance Search' and shows a search result for 'Substance (50-32-8)'. Under the heading 'Sources and type of information', there are two sections: 'Types' and 'Data sources'. The 'Types' section has checkboxes for Property information, Exposure and use information, and GHS classifications, all of which are checked. The 'Data sources' section has checkboxes for ACToR, APVMA-CR, Chemicals Dashboard, AGRITOX, CCR, ChemInfo, AICIS assessments, CESAR, and Combined Exposures, all of which are checked.

QUESTION 7

- Searches can be done for CLASSES of Chemicals too
- How many **explicit** chemicals are included in the class of chemicals “polychlorinated biphenyls”

302 211 209 104

Some example classes where we map data

- Classes of chemicals – what do we have?
 - PAHs, PCBs, PBDEs etc...
 - Strings and Substrings
 - InChI “first block” for skeleton
- Other “classes”
 - Similar chemicals
 - Related Substances
 - Lists of chemicals

QUESTION 7

- Searches can be done for CLASSES of Chemicals too
- How many **explicit** chemicals are included in the class of chemicals “polychlorinated biphenyls”

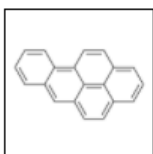
302

211

209

104

Similarity Searching



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Searched with a similarity threshold of 0.8

237 of 276 chemicals visible

Select all

Download

Send to Batch Search

Similarity



DTXSID

CASRN

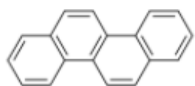
Similarity



Isotopes

Multicomponent Chemicals

Filter by Name or CASRN

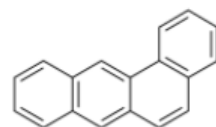


Chrysene

DTXSID:DTXSID0022432

CASRN:218-01-9

Similarity:1.00

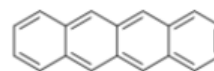


Benz(a)anthracene

DTXSID:DTXSID5023902

CASRN:56-55-3

Similarity:1.00

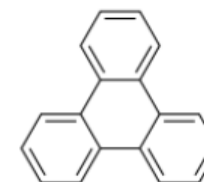


Naphthalene

DTXSID:DTXSID4059045

CASRN:92-24-0

Similarity:1.00

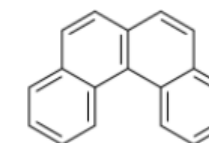


Triphenylene

DTXSID:DTXSID9059757

CASRN:217-59-4

Similarity:1.00



Benzo[c]phenanthrene

DTXSID:DTXSID4075459

CASRN:195-19-7

Similarity:1.00

QUESTION 8

- How many chemicals are “similar” in structure to ketoconazole with a threshold of >0.8 similarity (based on Tanimoto score).

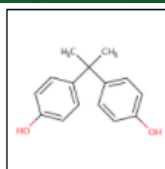
80

800

63

8

Related Substances



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

9 chemicals

Select all

Download

Send to Batch Search

Relationship



DTXSID

CASRN

TOXCAST

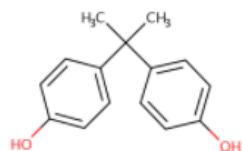


Hide chemicals that are:

Filter by Name or CASRN



Searched Chemical



[Bisphenol A](#)

DTXSID:DTXSID7020182

CASRN:80-05-7

TOXCAST:217/1152

Polymer

2 related chemical
structures with this
substance

[Formaldehyde, polymer with bisphenol A](#)

DTXSID:DTXSID3049627

CASRN:25085-75-0

TOXCAST:-

Polymer

2 related chemical
structures with this
substance

[Bisphenol A/ Epichlorohydrin resin](#)

DTXSID:DTXSID0050479

CASRN:25068-38-6

TOXCAST:-

Polymer

3 related chemical
structures with this
substance

[Bisphenol A-epichlorohydrin-polyformaldehyde](#)

DTXSID:DTXSID9050480

CASRN:28906-96-9

TOXCAST:-

Predecessor: Component

4 related chemical
structures with this
substance

[Fatty acids, C18-unsatd., dimers, polymers](#)

DTXSID:DTXSID40105886

CASRN:106906-26-7

TOXCAST:-

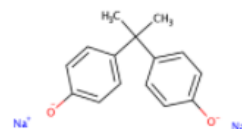
Predecessor: Component

3 related chemical
structures with this
substance

Predecessor: Component

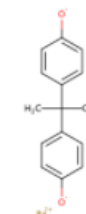
2 related chemical
structures with this
substance

Salt Form



[Disodium 4,4'-isopropylidenediphenolate](#)

Salt Form



[Barium\(2+\) 4,4'-isopropylidenebisphenolate](#)

QUESTION 8

- How many chemicals are “similar” in structure to ketoconazole with a threshold of >0.8 similarity (based on Tanimoto score).

80

800

63

8

Chemical Lists and Categories

Example: AEGLs list

Home Advanced Search Batch Search Lists ▼ Predictions Downloads

Lists of Chemicals

List of Assays

AEGLs: Acute Exposure Guideline Levels

Search AEGLVALUES Chemicals

☐ Identifier substring search

List Details

Description: Acute Exposure Guideline Level (AEGLs) values are intended to protect most individuals in the general population, including those that might be particularly susceptible to the harmful effects of the chemicals. Acute exposure guideline levels (AEGLs) describe the human health effects from once-in-a-lifetime, or rare, exposure to airborne chemicals. Used by emergency responders when dealing with chemical spills or other catastrophic exposures, AEGLs are set through a collaborative effort of the public and private sectors worldwide.

Number of Chemicals: 174

174 chemicals

Select all

Download ▼

Send to Batch Search

Name ▼

↑

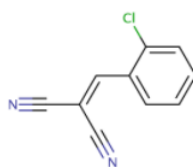
CASRN ✕

DTXSID ✕ ▼

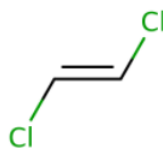
Hide chemicals that are: ▼

Filter by Name or CASRN

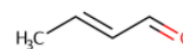
☰



(2-Chlorobenzylidene)propanedinitrile
CASRN:2698-41-1
DTXSID:DTXSID9020297



(E)-1,2-Dichloroethylene
CASRN:156-60-5
DTXSID:DTXSID7024031



(E)-Crotonaldehyde
CASRN:123-73-9
DTXSID:DTXSID6020351



(Z)-1,2-Dichloroethylene
CASRN:156-59-2
DTXSID:DTXSID2024030

PFAS lists of Chemicals

Select List

Download

Columns

PFAS

Copy Filtered Lists URL

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
EPAPFAS75S1	PFAS[EPA: List of 75 Test Samples (Set 1)]	2018-06-29	74	PFAS list corresponds to 75 samples (Set 1) submitted for initial testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program.
EPAPFAS75S2	PFAS[EPA: List of 75 Test Samples (Set 2)]	2019-02-21	75	PFAS list corresponds to a second set of 75 samples (Set 2) submitted for testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program.
EPAPFASCAT	PFAS[EPA Structure-based Categories]	2018-06-29	64	List of registered DSSTox "category substances" representing PFAS categories created using ChemAxon's Markush structure-based query representations.
EPAPFASINSOL	PFAS[EPA: Chemical Inventory Insoluble in DMSO]	2018-06-29	43	PFAS chemicals included in EPA's expanded ToxCast chemical inventory found to be insoluble in DMSO above 5mM.
EPAPFASINV	PFAS[EPA: ToxCast Chemical Inventory]	2018-06-29	430	PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing.
EPAPFASRL	PFAS[EPA: Cross-Agency Research List]	2017-11-16	199	EPAPFASRL is a manually curated listing of mainly straight-chain and branched PFAS (Per- & Poly-fluorinated alkyl substances) compiled from various internal, literature and public sources by EPA researchers and program office representatives.
PFASKEMI	PFAS: List from the Swedish Chemicals Agency (KEMI) Report	2017-02-09	2416	Perfluorinated substances from a Swedish Chemicals Agency (KEMI) Report on the occurrence and use of highly fluorinated substances.
PFASMASTER	PFAS Master List of PFAS Substances	2018-07-26	5061	PFASMASTER is a consolidated list of PFAS substances spanning and bounded by the below lists of current interest to researchers and regulators worldwide.
PFASOECD	PFAS: Listed in OECD Global Database	2018-05-16	4729	OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances, (PFASs) listing more than 4700 new PFAS
PFASTRIER	PFAS Community-Compiled List (Trier et al., 2015)	2017-07-16	597	PFASTRIER community-compiled public listing of PFAS (Trier et al, 2015)

QUESTION 9

- How many chemicals are in the EPA Toxics Release Inventory based on the associated list available on the dashboard?

666

677

766

777

Curated List of Pesticides

- Find list of interest

- Select list and send to batch

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads Share Search all data

Select List

PESTICIDES|EPA: Pesticide Chemical Search Database

Search EPAPCS Chemicals

☐ Identifier substring search

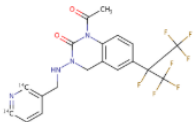
List Details

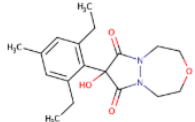
Description: The entries in this list have been classified in the U.S. as pesticidal "active ingredients" (conventional, antimicrobial, or biopesticidal agents), and were sourced from the Pesticide Chemical Search database (<https://iaspub.epa.gov/apex/pesticides/f?p=chemicalsearch:1>) created by EPA's Office of Pesticide Programs. Chemical Search provides a single point of reference for easy access to information previously published in a variety of locations, including various EPA web pages and Regulations.gov. Chemical search contains the following: 1) More than 20,000 regulatory documents; 2) Links to over 800 dockets in Regulations.gov 3) Links to pesticide tolerance (or maximum residue levels) information; 4) A variety of web services providing easy access to other scientific and regulatory information on particular chemicals from other EPA programs and federal government sources.

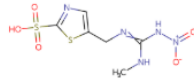
Number of Chemicals: 4012

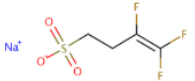
Select all Download **Send to Batch Search** CASRN DTXSID Mono.Mass 3988 chemicals

Hide chemicals that are: Filter by Name or CASRN


1-Acetyl-6-(1,1,1,2,3,3,3-heptafluoro-2-pyridyl)-4-methyl-2-pyridone
CASRN: NOCAS_920532
DTXSID: DTXSID00920532
Mono.Mass: 468.114807


8-(2,6-Diethyl-4-methylphenyl)-8-hydroxy-2,3-dihydro-1,4-benzodioxin-5-one
CASRN: NOCAS_920508
DTXSID: DTXSID10920508
Mono.Mass: 332.173607


5-(((Methylamino)(nitroamino)methylene)amino)-2-methylthiophene-3-sulfonic acid
CASRN: NOCAS_912338
DTXSID: DTXSID20912338
Mono.Mass: 295.004511


Sodium 3,4,4-trifluoro-3-buten-1-sulfonate
CASRN: NOCAS_912336
DTXSID: DTXSID00912336
Mono.Mass: 211.973094

- Singleton searches are great but...
- ...we generally want data on LOTS of chemicals!
- Typical questions
 - What are the structures for a set of chemical names? Set of CASRN's?
 - Can I get chemical lists in Excel files? As a list of SMILES strings?
Can I get an SDF file?
 - Can I include predicted properties in the download file? OPERA?
TEST?
 - Are “these chemicals” screened in Toxcast?
 - I’m a mass spectrometrists and need masses and formulae for a list of chemicals

QUESTION 9

- How many chemicals are in the EPA Toxics Release Inventory based on the associated list available on the dashboard?

666

677

766

777

Access data *en masse* for thousands of chemicals....

Batch Search ?



Step Three: Select Download Data or Display Chemicals

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.)

Sodium azide
O,O-Dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] phosphorodithioate
(Trichloromethyl)benzene
100-44-7
(Chloromethyl)benzene
98-07-7
111-44-4
1-Chloro-2-(2-chloroethoxy)ethane
Chloro(chloromethoxy)methane
2-(Butan-2-yl)-4,6-dinitrophenol

Display All Chemicals

Download Chemical Data

Select Output Format and Content

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

Select Output Format:







 Excel 

 Download






Customize Results

- ☐ Select All
- ☐ Select All in Lists






Chemical Identifiers

- ☒ DTXSID 
- ☒ Chemical Name 
- ☐ DTXCID 
- ☐ CAS-RN 
- ☐ InChIKey 
- ☐ IUPAC Name 













Structures

- ☐ Mol File 
- ☐ SMILES 
- ☐ InChI String 
- ☐ MS-Ready SMILES 
- ☐ QSAR-Ready SMILES 
















Intrinsic And Predicted Properties

- ☐ Molecular Formula 
- ☐ Average Mass 
- ☐ Monoisotopic Mass 
- ☐ TEST Model Predictions 
- ☐ OPERA Model Predictions 

Metadata

- ☐ Curation Level Details 
- ☐ NHANES/Predicted Exposure 
- ☐ Data Sources 
- ☐ Include ToxVal Data Availability 
- ☐ Assay Hit Count 
- ☐ Number of PubMed Articles 
- ☐ PubChem Data Sources 
- ☐ CPDat Product Occurrence Count 
- ☐ IRIS 
- ☐ PPRTV 
- ☐ Wikipedia Article
- ☐ QC Notes 
- ☐ Include links to ACToR reports - SLOW! (BETA) 

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 
- ☐ ARTICLE: Bench-Mark Dose Human Health Assessment List (Wignall et al., 2014) 
- ☐ ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (CERAPP) 
- ☐ ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (COMPARA) 
- ☐ ATSDR Toxicological Profiles 
- ☐ ATSDR: Minimal Risk Levels (MRLs) for Hazardous Substances 
- ☐ ATSDR: Toxic Substances Portal Chemical List 
- ☐ California Office of Environmental Health Hazard Assessment 
- ☐ Canadian Domestic Substances List 2019 
- ☐ CATEGORY: Amino acids 
- ☐ CATEGORY: Color Index dyes 
- ☐ CATEGORY: Flame Retardants 

Batch Search CASRN

Batch Search

Step 1

Step 2

Step 3







Step 4

Step 5






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

Please enter one identifier per line






Chemical Identifiers

- ☒ DTXSID 
- ☒ Chemical Name 
- ☐ DTXCID 
- ☒ CAS-RN 
- ☒ InChIKey 
- ☒ IUPAC Name 







Structures

- ☐ Mol File 
- ☐ SMILES 
- ☐ InChI String 
- ☒ MS-Ready SMILES 
- ☐ QSAR-Ready SMILES 

Intrinsic And Predicted Properties

- ☒ Molecular Formula 
- ☐ Average Mass 
- ☐ Monoisotopic Mass 
- ☐ TEST Model Predictions 
- ☒ OPERA Model Predictions 

Metadata






- ☐ Curation Level Details 
- ☐ NHANES/Predicted Exposure 
- ☐ Data Sources 
- ☒ Include ToxVal Data Availability 
- ☒ Assay Hit Count 
- ☒ Number of PubMed Articles 

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	INPUT	FOUND_BY	DTXSID	PREFERRED CASRN	INCHIKEY	IUPAC NAME	MOLECULAR WEIGHT	TOXVAL_D	TOXCAST	TOXCAST	MS_READY	NUMBER_CIRIS_LINK	PPRTV_LIN	ATMOSPHE	BIOCONCE		
2	534-52-1	CAS-RN	DTXSID10	2-Methyl-4,6	534-52-1	ZXVONLUN	2-Methyl-4,6	C7H6N2O5	Y	27.56	261/947	CC1=C(O)C	179	-	Y	1.571E-12	2.88959
3	115-21-9	CAS-RN	DTXSID70	Ethyl silicon	115-21-9	ZOYFEXPF	Trichloro(ethyl)	C2H5Cl3Si	Y	-	-	-	-	-	-	8.289E-12	13.9658
4	111-44-4	CAS-RN	DTXSID90	Bis(2-chloro	111-44-4	ZNSMNVML	1-Chloro-2-(C4H8Cl2O	Y	1.12	10/891	CICCOCCC	12	Y	-	2.647E-12	9.99608
5	2763-96-4	CAS-RN	DTXSID50	Muscimol	2763-96-4	ZJQHPWUV	5-(Aminome	C4H6N2O2	Y	-	-	NCC1=CC(C	4308	-	-	1.179E-10	5.05695
6	1464-53-5	CAS-RN	DTXSID00	2,2'-Bioxiran	1464-53-5	ZFIVKAOQ	2,2'-Bioxiran	C4H6O2	Y	-	-	C1OC1C1C	363	-	-	4.383E-12	1.27107
7	22224-92-6	CAS-RN	DTXSID30	Fenamiphos	22224-92-6	ZCJPOPBZ	Ethyl 3-methyl	C13H22NO3	Y	10.8	105/972	CCOP(=O)(C	58	Y	-	1.66E-11	2.3394
8	359-06-8	CAS-RN	DTXSID40	Fluoroacetyl	359-06-8	ZBHDYQJ	Fluoroacetyl	C2H2ClFO	Y	-	-	FCC(Cl)=O	-	-	-	3.513E-13	4.49379
9	5344-82-1	CAS-RN	DTXSID40	1-(o-Chloro	5344-82-1	YZUKKTCD	N-(2-Chloro	C7H7ClN2S	Y	-	-	NC(=S)NC1	-	-	-	2.482E-11	9.95206
10	7446-18-6	CAS-RN	DTXSID10	Thallium (I)	7446-18-6	YTQVHRVI	Dithallium(1-	O4STI2	Y	-	-	-	34	Y	Y	-	-
11	62207-76-5	CAS-RN	DTXSID40	Bis(3-fluoro	62207-76-5	YRZXYIHD	-	C16H14CoF	Y	-	-	-	-	-	-	-	-
12	66-81-9	CAS-RN	DTXSID60	Cycloheximi	66-81-9	YPHMISFO	4-[(2R)-2-[(C15H23NO4	Y	32.27	294/911	CC1CC(C)C	18709	-	-	1.756E-11	2.81761
13	106-96-7	CAS-RN	DTXSID30	Propargyl bi	106-96-7	YORCIIVHU	3-Bromopro	C3H3Br	Y	-	-	BrCC#C	-	-	-	1.069E-11	10.4968
14	315-18-4	CAS-RN	DTXSID70	Mexacarbat	315-18-4	YNEVBPNZ	4-(Dimethyl	C12H18N2C	Y	5.11	12/235	CNC(=O)OC	27	-	-	1.447E-11	26.2914
15	110-00-9	CAS-RN	DTXSID60	Furan	110-00-9	YLQBMQCI	Furan	C4H4O	Y	0.0	0/235	O1C=CC=C	919	Y	-	4.019E-11	5.01648
16	3037-72-7	CAS-RN	DTXSID20	4-(diethoxy	3037-72-7	YHFFINXFN	4-[Diethoxy(C9H23NO2	Y	-	-	-	-	-	-	5.95E-12	6.71292
17	75-44-5	CAS-RN	DTXSID00	Phosgene	75-44-5	YGYAWVD	Carbonyl dic	CCl2O	Y	-	-	ClC(Cl)=O	489	Y	-	9.994E-16	13.0711
18	2032-65-7	CAS-RN	DTXSID30	Methiocarb	2032-65-7	YFBPRJGD	3,5-Dimethy	C11H15NO2	Y	18.14	88/485	CNC(=O)OC	65	-	-	1.446E-11	34.1692
19	2778-04-3	CAS-RN	DTXSID20	Endothion	2778-04-3	YCAGGFXS	[(5-Metho	C9H13O6P	Y	-	-	COC1=COCC	-	-	-	4.355E-11	1.18341
20	12108-13-3	CAS-RN	DTXSID90	(Methylcyc	12108-13-3	YASXMYPV	Tricarbonyl(C9H7MnO3	Y	2.56	11/430	-	68	-	-	-	-
21	7803-51-2	CAS-RN	DTXSID20	Phosphine	7803-51-2	XYFCBTPG	Phosphane	H3P	Y	-	-	-	928	Y	-	-	-
22	107-18-6	CAS-RN	DTXSID80	Allyl alcohol	107-18-6	XXROGKLT	Prop-2-en-1	C3H6O	Y	3.99	17/426	OCC=C	627	Y	Y	2.592E-11	4.03901
23	108-05-4	CAS-RN	DTXSID30	Vinyl acetat	108-05-4	XTXRWKR	Ethethyl acet	C4H6O2	Y	1.7	4/235	CC(=O)OC	206	Y	-	2.5E-11	5.52157
24	19624-22-7	CAS-RN	DTXSID10	Pentaborane	19624-22-7	XPIBKKWN	-	B5H9	Y	-	-	-	-	-	-	-	-
25	75-74-1	CAS-RN	DTXSID00	Tetramethyl	75-74-1	XOOGZRUE	Tetramethyl	C4H12Pb	Y	-	-	C[Pb](C)(C)	24	-	-	-	-











Worksheet1

Send to batch and select....

Intrinsic And Predicted Properties

- ☐ Molecular Formula 
- ☐ Average Mass 
- ☐ Monoisotopic Mass 
- ☐ TEST Model Predictions 
- ☐ OPERA Model Predictions 

Metadata

- ☐ Curation Level Details 
- ☐ NHANES/Predicted Exposure 
- ☐ Data Sources 
- ☐ Include ToxVal Data Availability 
- ☐ Assay Hit Count 
- ☐ Number of PubMed Articles 
- ☐ PubChem Data Sources 
- ☐ CPDat Product Occurrence Count 
- ☐ IRIS 
- ☐ PPRTV 

- A few seconds to assemble
 - ToxCast data - #actives/#assays and % active
 - # articles in PubMed
 - Links to IRIS or PPRTV reports
 - TEST or OPERA predictions
 - Exposure data: predictions and CPDat

A	B	C	D	E	F	G	H	I	J	K	L	M
DTXSID	PREFERRED_NAME	EXPOCAST_ME	EXPOCAST_NH	ANES	TOXVAL_DATA	TOXCAST_%_ACT	TOXCAST_	#PUBMED	PUBCHEM_	CPDAT_COU	IRIS_LINK	PPRTV_LINK
DTXSID2021105	Pentachloronitrobenzene	1.14e-07	Y	Y	Y	11.8	99/839	69	96	164	Y	-
DTXSID4022527	Propylparaben	1.4e-05	Y	Y	Y	13.77	99/719	201	121	1476	-	-
DTXSID4024064	Dinex	8.29e-08	Y	-	Y	42.13	99/235	-	35	5	Y	-
DTXSID0032493	Triadimenol	1.73e-08	Y	-	Y	10.54	98/930	163	74	83	-	-
DTXSID4032667	Esfenvalerate	1.7e-06	Y	-	Y	11.45	98/856	483	45	198	-	-
DTXSID6020561	Endrin	1.29e-07	Y	-	Y	14.02	98/699	284	16	98	Y	Y
DTXSID6025355	Glutaraldehyde	2.03e-05	Y	-	Y	14.35	98/683	6515	139	1144	-	-
DTXSID8032417	Isofenphos	1.87e-08	Y	-	Y	16.28	98/602	30	42	60	-	-
DTXSID6032352	Chlorpyrifos-methyl	1.07e-07	Y	Y	Y	11.27	97/861	72	50	116	-	-
DTXSID8020620	Fenthion	8.99e-08	Y	Y	Y	11.56	97/839	354	100	99	-	-
DTXSID2020189	FD&C Blue No. 1	0.000178	Y	-	Y	13.72	97/707	174	49	672	-	-
DTXSID7044843	Erythrosin B	6.3e-07	Y	-	-	24.25	97/400	14843	51	7	-	-
DTXSID5041778	Chloropropylate	1.05e-07	Y	-	Y	40.93	97/237	-	36	12	-	-
DTXSID5023900	Benomyl	1.11e-07	Y	-	Y	11.23	96/855	476	91	105	Y	-
DTXSID9020247	Carbaryl	5.61e-08	Y	Y	Y	11.51	96/834	1135	117	245	Y	-
DTXSID8024109	Flutolanil	1.63e-08	Y	-	Y	11.4	95/833	6	59	80	-	-
DTXSID1023998	Cypermethrin	1.62e-06	Y	Y	Y	10.78	94/872	1148	148	246	-	-
DTXSID2024242	Paclobutrazol	9.19e-08	Y	-	Y	11.11	94/846	139	-	40	Y	-
DTXSID1020807	2-Mercaptobenzothiazole	4.7e-05	Y	-	Y	12.82	94/733	111	181	86	-	Y

QUESTION 10

- How many chemicals are in the Tox21 Screening library, based on the **associated dashboard list**

4987 6587 8947 7632

- *What is the Tox21 Screening Library?? How is it valuable? **NEXT TIME***

In the next Session we discuss NAMS



Wednesday, Aug. 18, 2021 | 1:00–3:00 p.m. (Central US Time)

"NEW APPROACH METHODS"—WHAT IS THAT?

- An introduction to New Approach Methods
 - What's a NAM?
 - *In silico* – QSAR and read-across
 - *In vitro* assays
 - *In vitro* toxicokinetics
 - Computer modeling
- Short introduction to QSAR model data in the Dashboard
 - TEST predictions
 - OPERA predictions
 - Calculation reports
 - Realtime prediction
- An introduction to ToxCast and Tox21
- An overview of assay endpoints and biology

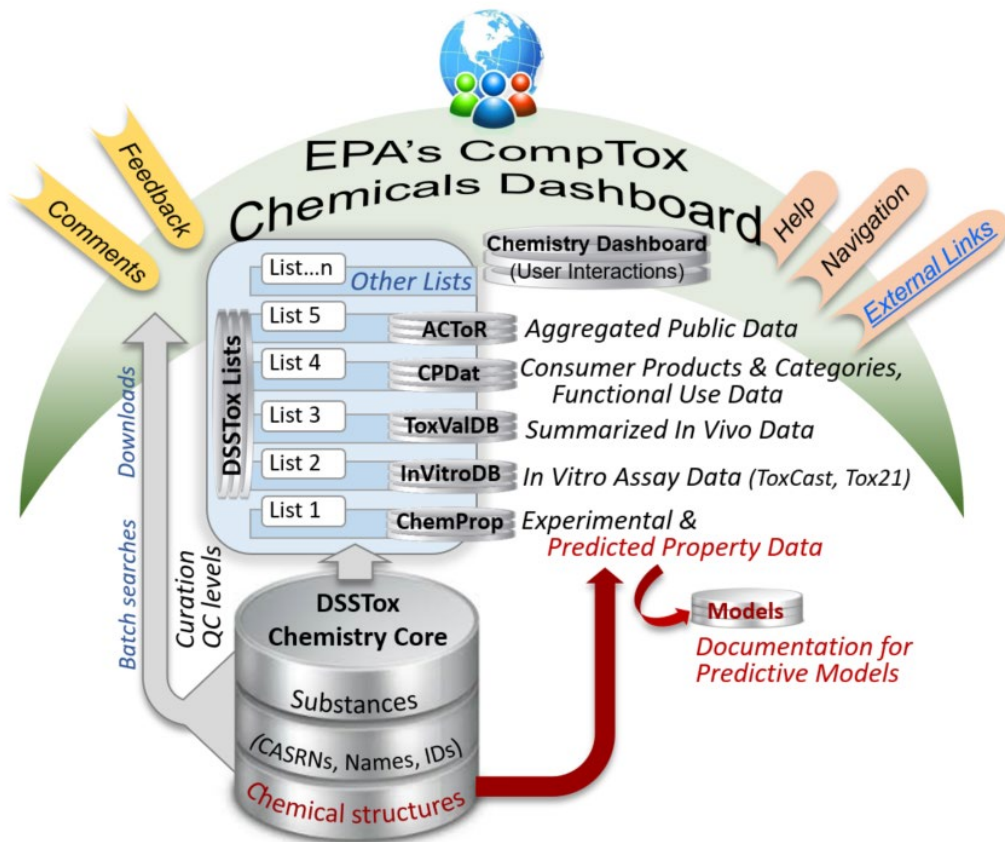


QUESTION 10

- How many chemicals are in the Tox21 Screening library, based on the associated dashboard list

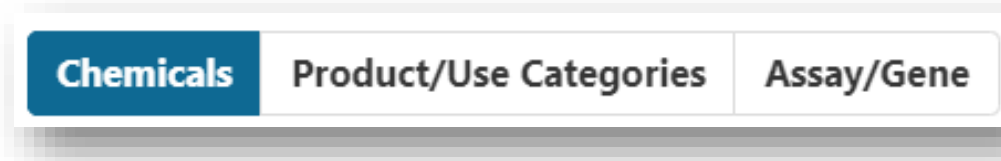
4987 6587 8947 7632

Summary and Conclusion



- CompTox Chemicals Dashboard - a central hub for environmental data


- ~875k chemical substances
- Integrating property data, hazard data, exposure data, *in vitro* bioactivity data
- Interrogation of bioactivity data -
- Multiple types of searches




- Batch search for thousands of chemicals
- Real-time property and toxicity predictions
- Downloadable files – CSV, TSV and Excel

Summary and Conclusions


- The Dashboard is one of *many* applications on the internet from which you can source data
- It is not difficult to do a Google search on get some form of answer
- Always question the data, and sometimes even “facts”
- We work hard to qualify, curate and validate data but obtain some from public sources



United States
Environmental
Assessment
Center



DHMO.org
Dihydrogen Monoxide
Research Division




Support the
cause! Visit the
DHMO.org
Store

VISA PayPal MasterCard

FAQs

- [What is Dihydrogen Monoxide?](#)
- [Should I be concerned about Dihydrogen Monoxide?](#)
- [Why haven't I heard about Dihydrogen Monoxide before?](#)
- [What are some of the dangers associated with DHMO?](#)
- [What are some uses of Dihydrogen Monoxide?](#)
- [What is the link](#)

Dihydrogen Monoxide FAQ



Frequently Asked Questions About Dihydrogen Monoxide (DHMO)

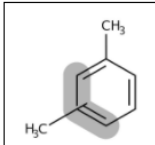
What is Dihydrogen Monoxide?

Dihydrogen Monoxide (DHMO) is a colorless and odorless chemical compound, also referred to by some as Dihydrogen Oxide, Hydrogen Hydroxide, Hydronium Hydroxide, or simply Hydric acid. Its basis is the highly reactive hydroxyl radical, a species shown to mutate DNA, denature proteins, disrupt cell membranes, and chemically alter critical neurotransmitters. The atomic components of DHMO are found in a number of caustic, explosive and poisonous

If you find an error, or want to comment...

Select text and "Submit Comment"

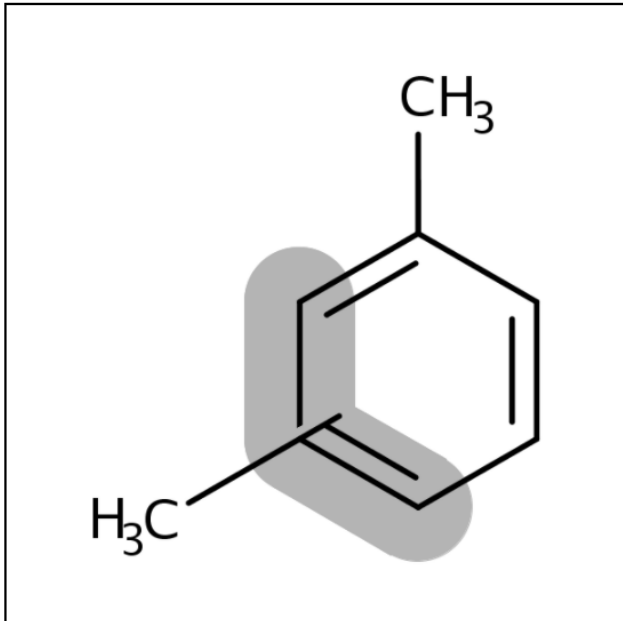
[Home](#) [Advanced Search](#) [Batch Search](#) [Lists](#) [Predictions](#) [Downloads](#) [Copy](#) [Share](#) [Submit Comment](#)



Xylenes

1330-20-7 | DTXSID2021446

Searched by DSSTox Substance Id.



Wikipedia

Xylene (from Greek ξύλον *xylon*, "wood"), **xylol** or **dimethylbenzene** is any one of the three isomers of dimethylbenzene, or a combination thereof. With the formula $(\text{CH}_3)_2\text{C}_6\text{H}_4$, each of the three isomers consists of a central benzene ring with two methyl groups attached at substituents. They are all colorless liquids with a sweet odor, and are of great industrial value.




...



[Read more](#)


Quality Control Notes

Ill-defined substance;

Intrinsic Properties

 **Molecular Formula:** Not Found  Mol File  Find All Chemicals

 **Average Mass:** 0 g/mol  Isotope Mass Distribution

 **Monoisotopic Mass:** 0 g/mol

New Comment

Details to be submitted with your comment

Text selected: 1330-20-7

Found On: July 14th 2021, 7:08:59 am

Original Query: /dsstoxdb/results?search=DTXSID2021446


Browser: Chrome 91

Comment

This does not match the CASRN I have for Xylene. I have 95-47-6. Are you sure your CASRN is correct?

Email address

williams.antony@epa.gov

 I'm not a robot



[Submit](#)

comptox.epa.gov says

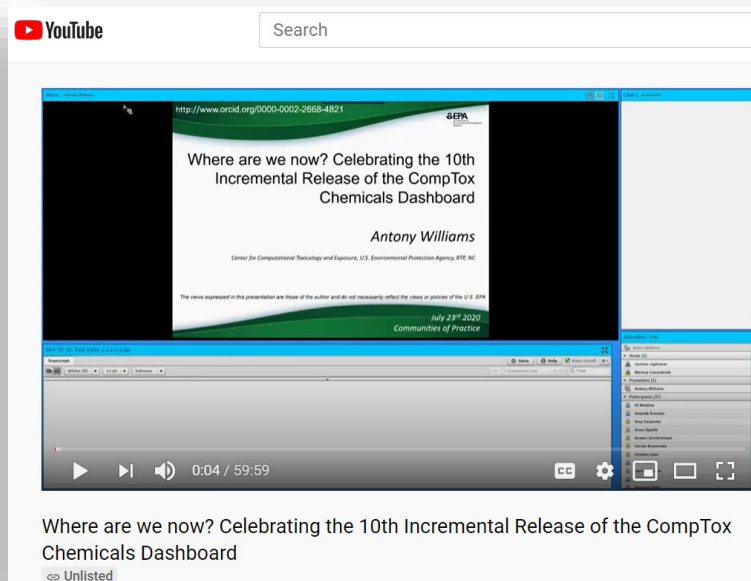
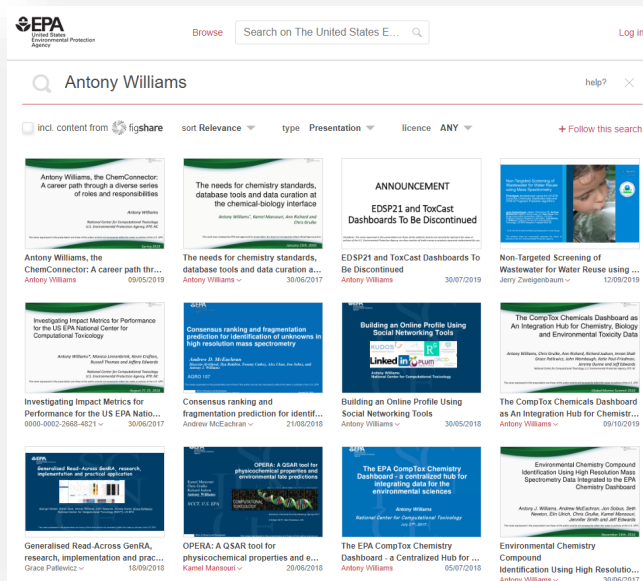
Your comment has been submitted and will be reviewed.

[OK](#)

- The CompTox Chemistry Dashboard: a community data resource for environmental chemistry, *J. Cheminformatics*, **9**, 61 (2017)
- EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research, *Comp. Tox.* **12**, 100096 (2019)
- OPERA models for predicting physicochemical properties and environmental fate endpoints, *J. Cheminformatics*, **10**, 10 (2018)
- Screening Chemicals for Estrogen Receptor Bioactivity Using a Computational Model, *Environ. Sci. Technol.* **49**, 8804-8814 (2015)
- ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology, *Chem. Res. Toxicol.* **29**, 1225-51 (2016)
- Development and Validation of a Computational Model for Androgen Receptor Activity, *Chem. Res. Toxicol.* **30**, 946-964 (2017)
- CERAPP: Collaborative Estrogen Receptor Activity Prediction Project, *Environ. Health Perspect.* **124**, 1023 (2016)
- Abstract Sifter: a comprehensive front-end system to PubMed, *F1000*, **6**, 2164 (2017)

You want to know more...

- Lots of resources available
 - Presentations: <https://tinyurl.com/w5hq55>
 - Communities of Practice Videos: <https://rb.gy/qsbn01>
 - Manual: <https://rb.gy/4fgydc>
 - Latest News: https://comptox.epa.gov/dashboard/news_info

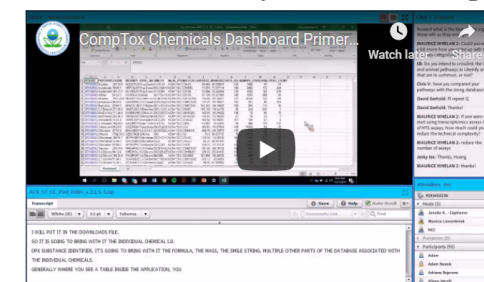


CompTox Chemicals Dashboard primer videos

The CompTox Chemicals Dashboard is a one-stop-shop for chemistry, toxicity and exposure information for over 875,000 chemicals. Data and models within the Dashboard also help with efforts to identify chemicals of most need of further testing and reducing the use of animals in chemical testing.

Explore the wealth of data and features available in the CompTox Chemicals Dashboard with these instructional videos narrated by EPA scientists.

General Chemistry and Search Capabilities



Acknowledgments

- Contact: Williams.Antony@epa.gov
- Feedback and follow-up is welcomed! Your questions help
- The dashboard is based on the efforts of many more team members than us. Many collaborators provide data also.



EPA's Center for Computational Toxicology and Exposure



Thank you for joining us !

Next Session:

Wednesday August 18, 2021 1:00 – 3:00 pm (Central US Time)

“New Approach Methods – What is That?”

Antony Williams – US Environmental Protection Agency

