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EPA United States Environmental Protection Agency

US-EPA Chemicals Dashboard – an integrated data hub for environmental science

Antony John Williams

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

May 5th 2021 : Lehman College

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

Agenda

- Short overview of the ***CompTox Chemicals Dashboard***
- Live demo – please ask questions as we go!!!

- ***SLIDES WILL BE MADE AVAILABLE AT THE END***

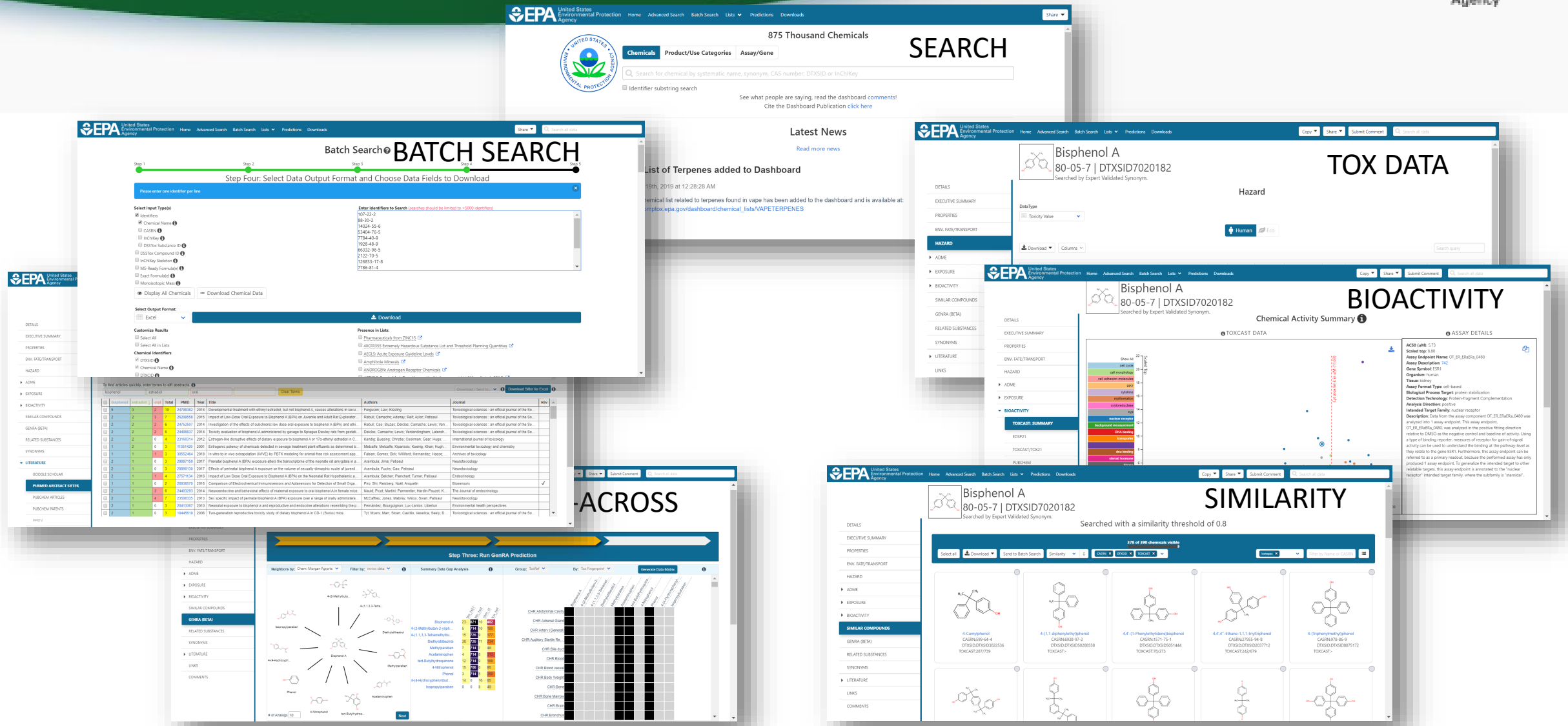
CompTox Chemicals Dashboard
https://comptox.epa.gov/dashboard

- A **publicly accessible website** delivering access:

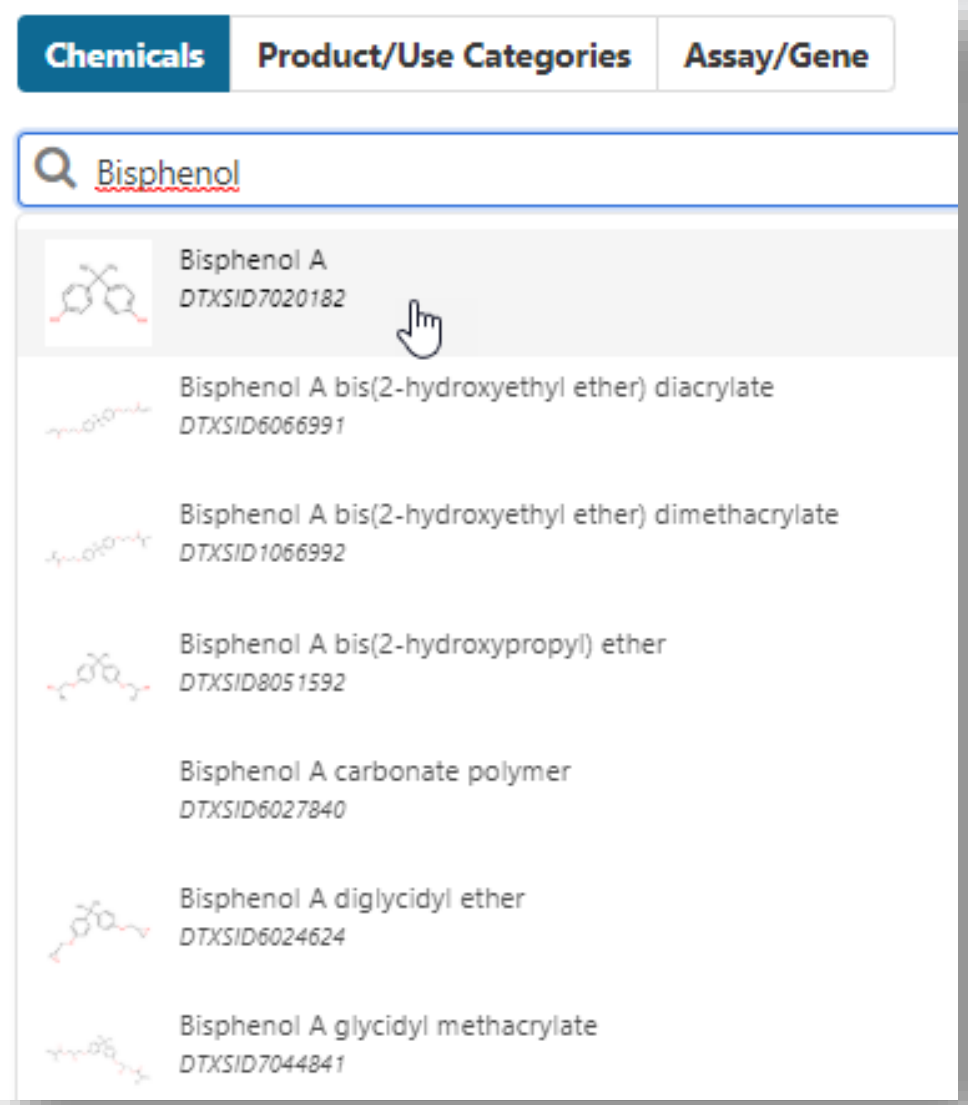
  - ~883,000 chemicals with related property data
  - Experimental and predicted physicochemical property data
  - Experimental Human and Ecological hazard data
  - Integration to “biological assay data” for 1000s of chemicals
  - Information regarding consumer products containing chemicals
  - Links to other agency websites and public data resources
  - “Literature” searches for chemicals using public resources
  - “Batch searching” for thousands of chemicals

CompTox Chemicals Dashboard

https://comptox.epa.gov/dashboard



BASIC Search

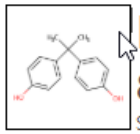


- Three searches from the home page
  - Chemicals (Names, CASRN, Substring)
  - Product/Use Categories
  - Assay Gene
- Searching millions of synonyms and includes Active, Deleted and Alternate CASRNs

Detailed Chemical Pages

EPA United States Environmental Protection Agency

EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Copy | Share | Submit Comment | Search all data

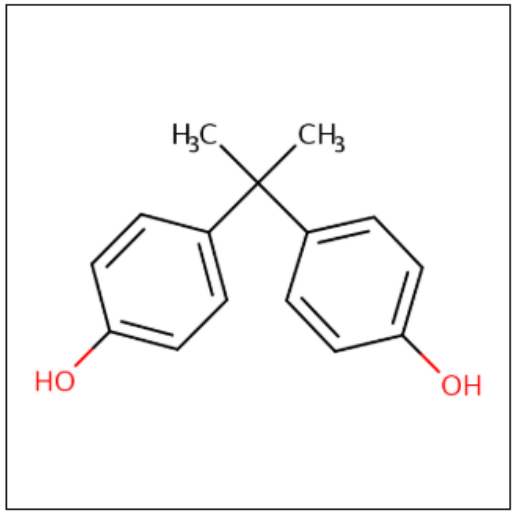


Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

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



Wikipedia

Bisphenol A (**BPA**) is an organic synthetic compound with the chemical formula $(CH_3)_2C(C_6H_4OH)_2$ belonging to the group of diphenylmethane derivatives and bisphenols, with two hydroxyphenyl groups. It is a colorless solid that is soluble in organic solvents, but poorly soluble in water (0.344 wt % at 83 °C).
BPA is a starting material for the synthesis of plastics, primarily certain polycarbonates
...
Read more

Intrinsic Properties

Molecular Formula: $C_{15}H_{16}O_2$ | Mol File | Find All Chemicals

Average Mass: 228.291 g/mol | Isotope Mass Distribution

Monoisotopic Mass: 228.11503 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Quality Control Notes

Lists of Lists of Chemicals
>290 lists and growing

EPA United States Environmental Protection Agency

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

Lists of Chemicals
List of Assays

Select List

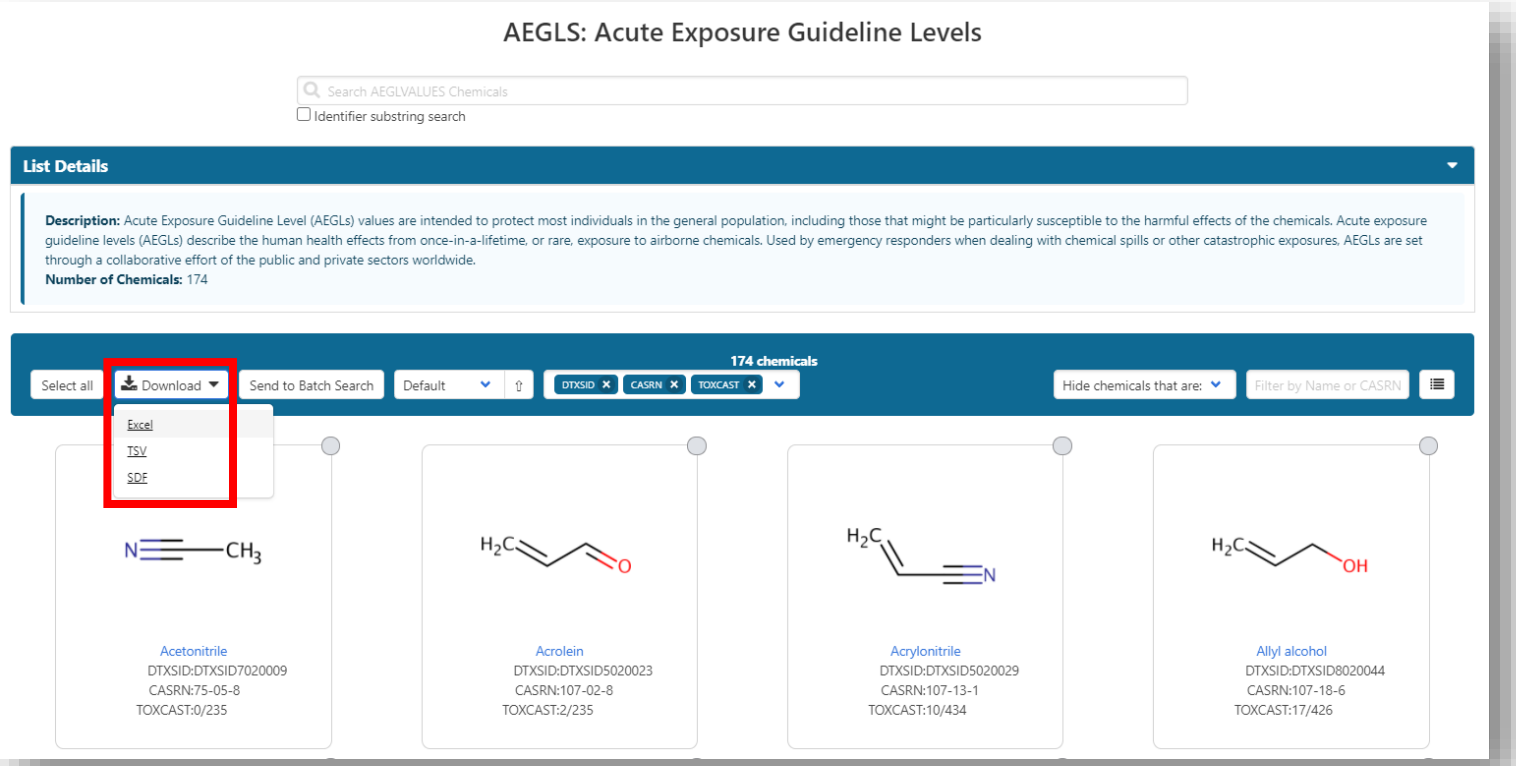
Download | Columns | 10 | Search query | Copy page URL

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
40CFR1164	40CFR116.4 Designation of Hazardous Substances (Above Ground Storage Tanks)	2020-06-25	331	Hazardous Substance List (40CFR116.4): related to Above Ground Storage Tanks
40CFR355	40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities	2018-01-05	354	Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378)
ACSREAG	LIST: ACS Reagent Chemicals	2017-04-14	405	The ACS Committee on Analytical Reagents sets purity specifications for almost 500 reagent chemicals and over 500 standard-grade reference materials.
AEGLVALUES	AEGLS: Acute Exposure Guideline Levels	2018-04-20	174	Acute exposure guideline levels (AEGLs) describe the human health effects from once-in-a-lifetime, or rare, exposure to airborne chemicals.
ALGALTOX	LIST: Algal Toxins	2018-05-04	55	A list of Algal Toxins of potential interest
AMINOACIDS	CATEGORY: Amino acids	2019-02-04	20	Amino acids are organic compounds containing amine (-NH2) and carboxyl (-COOH) functional groups, along with a side chain (R group) specific to each amino acid.
AMPHIBOLES	LIST: Amphiboles	2019-03-26	23	Amphiboles are an important group of inosilicate minerals.
ANTIBIOTICS	CATEGORY|PHARMACEUTICALS: Antibiotics	2019-11-16	170	List of antibiotics and related compounds
ANTIMICROBIALS	CATEGORY|WIKILIST|ANTIMICROBIALS: List of Antimicrobials from Wikipedia	2020-10-11	289	A list of antimicrobials extracted from Wikipedia.
AOPSTRESSORS	List of Adverse Outcome Pathway Stressors	2020-06-05	349	List of Adverse Outcome Pathway Stressors from the AOP Database

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

Showing 1 to 10 of 281 records

List of Chemicals
Example: Acute Exposure Guideline Levels



- Chemical List Examples
  - Disinfection by-products
  - EPA Pesticide Search DB
  - Consumer Products DB
  - Chemicals in Biosolids
  - ATSDR Toxicological Profiles
  - Canadian Domestic Substances
  - Chemical Inventory for ToxCast
  - EFSA OpenFoodTox
  - EDSP Universe of Chemicals
  - Hydraulic Fracturing Chemicals

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 c

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

Level 3: Programmatically curated from high quality EPA source, unique chemical i

Level 4: Programmatically curated from ChemID, unique chemical identifiers have r

Level 5: Programmatically curated from ACToR or PubChem, unique chemical ident

Computational Toxicology 12 (2019) 100096

Contents lists available at ScienceDirect

Computational Toxicology

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

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

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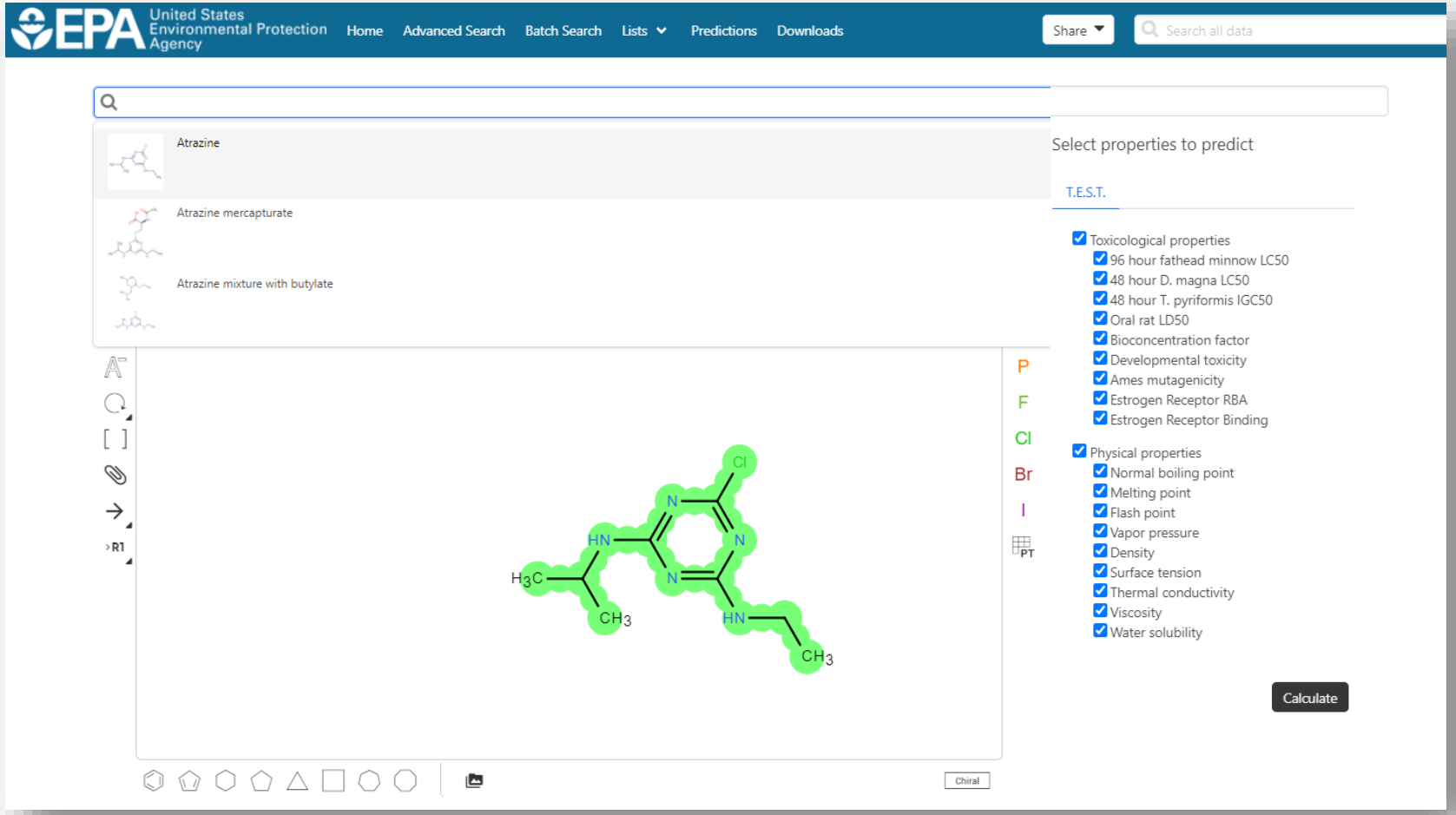
Predictions for New Chemicals

https://comptox.epa.gov/dashboard/predictions/index



Predictions for New Chemicals

https://comptox.epa.gov/dashboard/predictions/index

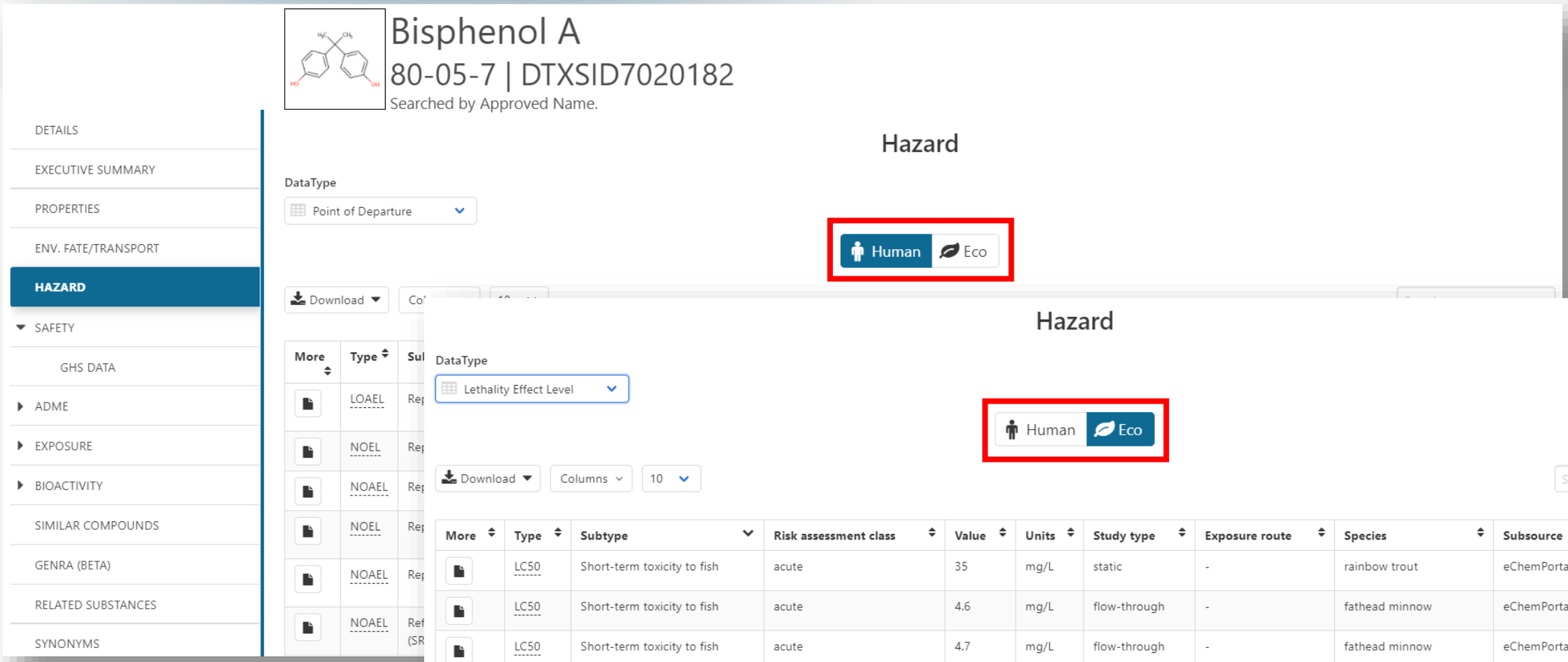
EPA United States Environmental Protection Agency

Provider: T.E.S.T.

Download Summary

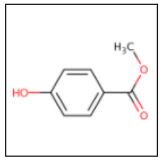
Property	Experimental Value	Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50		3.969 -Log10(mol/L) 22.469 mg/L	3.936 -Log10(mol/L) 24.234 mg/L	3.742 -Log10(mol/L) 37.882 mg/L	4.135 -Log10(mol/L) 15.355 mg/L	4.064 -Log10(mol/L) 18.079 mg/L
48 hour D. magna LC50		3.791 -Log10(mol/L) 33.887 mg/L	3.568 -Log10(mol/L) 56.592 mg/L	4.243 -Log10(mol/L) 11.976 mg/L	3.832 -Log10(mol/L) 30.824 mg/L	3.521 -Log10(mol/L) 63.123 mg/L
48 hour T. pyriformis IGC50			2.986 -Log10(mol/L) 216.359 mg/L			
Oral rat LD50		2.439 -Log10(mol/kg) 761.182 mg/kg	2.355 -Log10(mol/kg) 924.254 mg/kg			2.524 -Log10(mol/kg) 626.882 mg/kg
Bioconcentration factor		0.847 Log10 7.038	0.906 Log10 8.051	0.690 Log10 4.903	0.820 Log10 6.607	0.974 Log10 9.409
Developmental toxicity		true	true	true		
Ames mutagenicity		false	true			false
Estrogen Receptor RBA						
Estrogen Receptor Binding		false	false	false	false	
Normal boiling point		315.9 °C	318.0 °C		345.4 °C	284.3 °C
Melting point		114.0 °C	105.0 °C		79.4 °C	157.7 °C
Flash point		176.1 °C	180.1 °C		172.5 °C	175.7 °C
Vapor pressure		-6.072 Log10(mmHg) 8.464*10^-7 mmHg	-6.164 Log10(mmHg) 6.851*10^-7 mmHg		-5.679 Log10(mmHg) 2.093*10^-6 mmHg	-6.374 Log10(mmHg) 4.23*10^-7 mmHg

Hazard Data (Human and Eco)



Sources of Exposure to Chemicals

EPA United States Environmental Protection Agency



Methylparaben

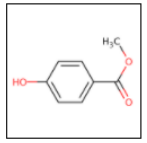
99-76-3 | DTXSID4022529

Searched by DSSTox Substance Id.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- SAFETY
- ADME
- EXPOSURE
  - PRODUCT & USE CATEGORIES
  - CHEMICAL WEIGHT FRACTION
  - CHEMICAL FUNCTIONAL USE
  - TOXICS RELEASE INVENTORY

Product and Use Categories (PUCs)

Download | Columns | 10 | Search query



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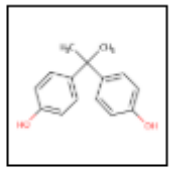
- EXPOSURE
  - PRODUCT & USE CATEGORIES
  - CHEMICAL WEIGHT FRACTION
  - CHEMICAL FUNCTIONAL USE
  - TOXICS RELEASE INVENTORY
  - MONITORING DATA

Chemical Weight Fractions

Download | Columns | 25 | Search query

Product Name	Product Use Category	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source
YOUTOPIA- PET SHAMPOO	all pets: pet shampoo			MSDS	CPCPdb
YLP Lip Gloss Solid F4203-06006-A12	make-up and related: lip gloss			MSDS	CPCPdb
ylp lip gloss liquid multiple colors 2	make-up and related: lip gloss			MSDS	CPCPdb
YLP Lip Gloss Liquid F4204-06001-A47	make-up and related: lip gloss			MSDS	CPCPdb
YLP Lip Gloss Liquid F4204-06001-A21	make-up and related: lip gloss			MSDS	CPCPdb
wondermask p peelable mask_ 2211 bulk	Not Yet Categorized:	0.00	1.00e-2	MSDS	SIRI
waterlss skn cleansr w/plastc scrubr_sbs-33	Not Yet Categorized:			MSDS	SIRI
water for injection_ bacteriostatic	Not Yet Categorized:			MSDS	SIRI
Water Based Nail Polish - 196C	nails: nail polish			other	CPCPdb
Washable Ink	Not Yet Categorized:			MSDS	CPCPdb
Vitamin Cream	facial cleansing and moisturizing: face cream/moisturizer			MSDS	CPCPdb

Identifiers to Support Searches



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.

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

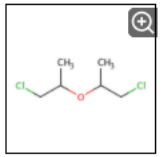
Synonyms

Download | 25 | Search query

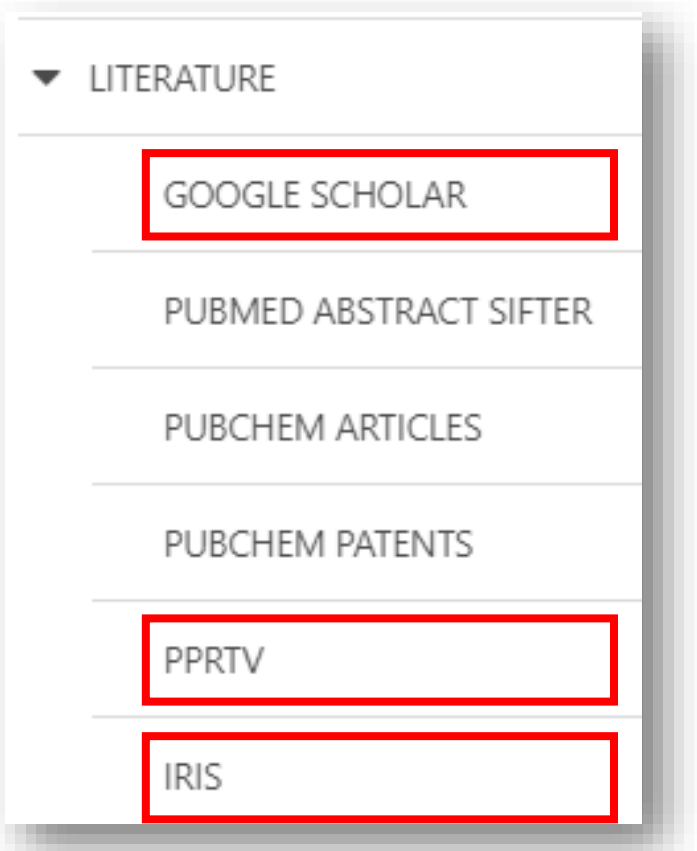
Synonym	Quality
Bisphenol A	**Valid**
4,4'-(Propane-2,2-diyl)diphenol	**Valid**
Phenol, 4,4'-(1-methylethylidene)bis-	**Valid**
80-05-7 Active CAS-RN	**Valid**
BPA	**Valid**
4,4'-Propane-2,2-diyldiphenol	**Valid**
Phenol, 4,4'-(1-methylethylidene)bis-	**Valid**
4-06-00-06717 Beilstein Registry Number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

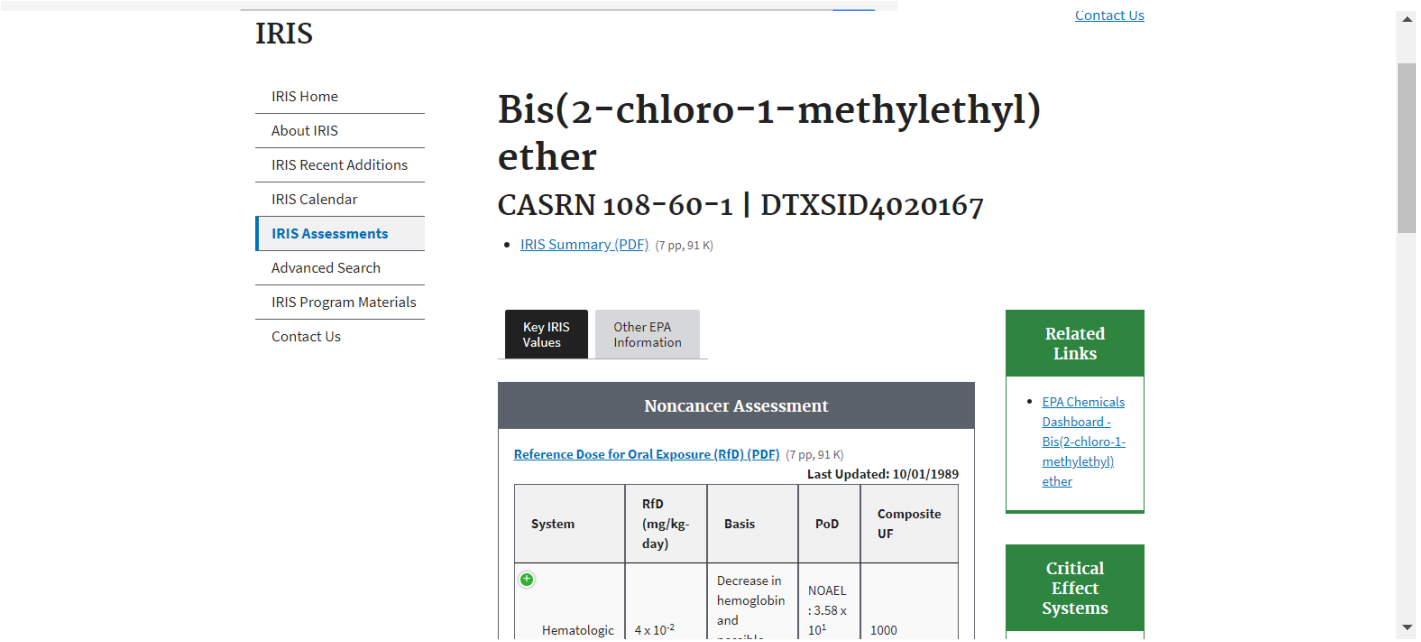
Identifiers are used in the app

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

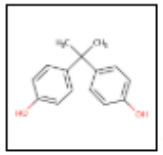


bis(2-Chloro-1-methylethyl) ether
108-60-1 | DTXSID4020167





External Links – Also use Identifiers Names, CASRN, PubChem IDs…



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- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- **LINKS**
- COMMENTS

General

- EPA Substance Registry Service
- Household Products Database
- Chemical Entities of Biological Interest (ChEBI)
- PubChem
- Chemspider
- CPCat
- DrugBank
- HMDB
- Wikipedia
- MSDS Lookup
- ChEMBL
- Chemical Vendors
- CalEPA Office of Environmental Health Hazard Assessment
- NIOSH Chemical Safety Cards
- ToxPlanet
- ACS Reagent Chemicals
- Wikidata
- ChemHat: Hazards and Alternatives Toolbox
- Wolfram Alpha
- ScrubChem
- ECHA Brief Profile

Toxicology

- ACToR
- DrugPortal
- CCRIS
- ChemView
- CTD
- eChemPortal
- Gene-Tox
- HSDB
- ToxCast Dashboard 2
- LactMed
- International Toxicity Estimates for Risk
- ATSDR Toxic Substances Portal
- Superfund Chemical Data matrix
- NIOSH IDLH Values
- ACToR PDF Report
- Toxics Release Inventory
- CREST
- National Air Toxics Assessment

Publications

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

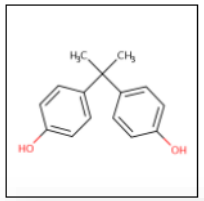
Analytical

- FOR-IDENT
- NEMI: National Environmental Methods Index
- RSC Analytical Abstracts
- Tox21 Analytical Data
- MONA: MassBank North America
- mzCloud
- NIST IR Spectrum
- NIST MS Spectrum

Prediction

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

External Links



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

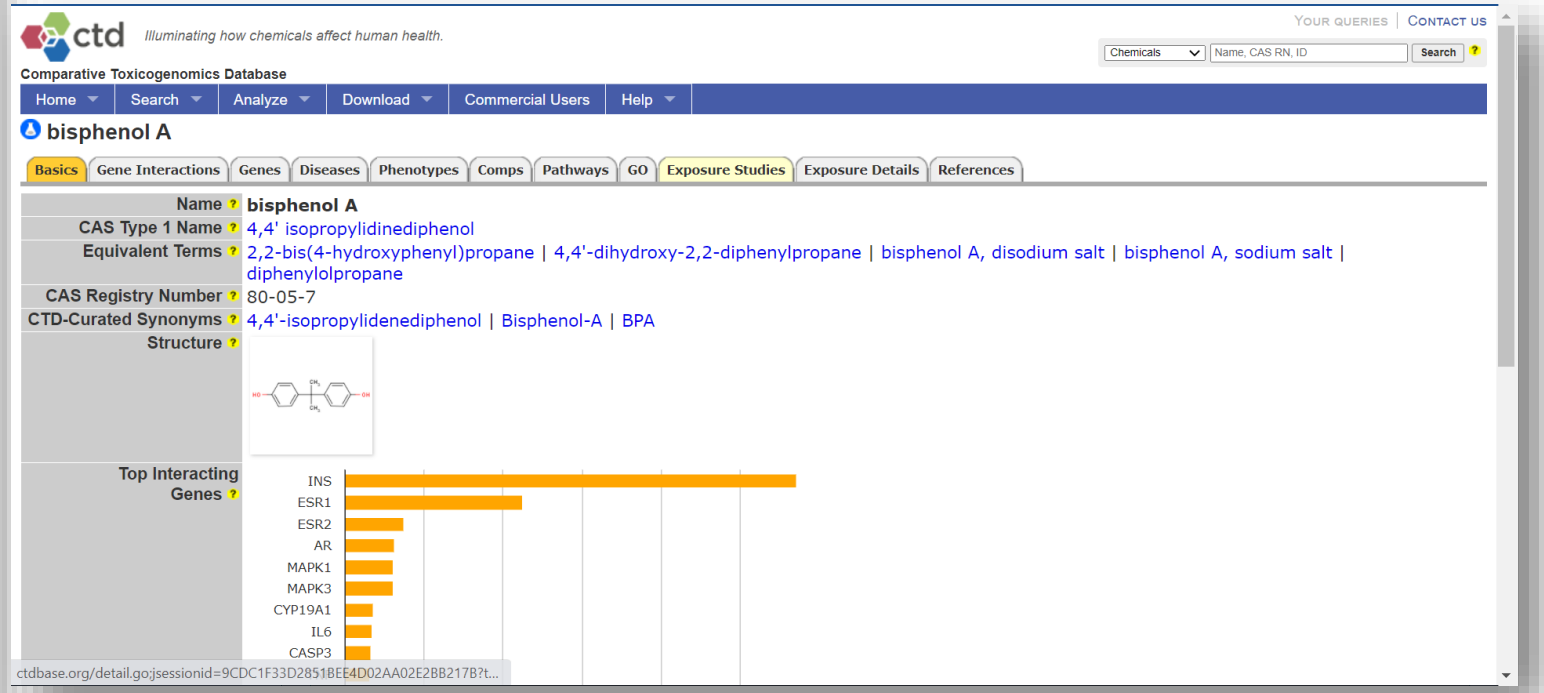
General

- EPA Substance Registry Service
- PubChem
- Chemspider
- CPCat
- DrugBank
- Wikipedia
- MSDS Lookup
- ChEMBL
- ToxPlanet
- ACS Reagent Chemicals
- ChemHat: Hazards and Alternatives Toolbox

Toxicology

- ACToR
- DrugPortal
- CCRIS
- ChemView
- CTD
- eChemPortal
- Gene-Tox
- HSDB
- ToxCast Dashboard 2
- ACToR PDF Report
- CREST
- National Air Toxics Assessment

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



Batch Searching

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

EPA United States Environmental Protection Agency

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

Batch Search

Step 1 — Step 2 — Step 3 — Step 4 — Step 5

Step Three: Select Download Data or Display Chemicals

Please enter one identifier per line

Select Input Type(s)

- [x] Identifiers
  - [x] Chemical Name
  - [x] 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

EPA United States Environmental Protection Agency

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

- [x] DTXSID
- [x] 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 CASRNs

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
- [x] DTXSID
- [x] Chemical Name
- [ ] DTXCID
- [x] CAS-RN
- [x] InChIKey
- [x] IUPAC Name

Structures
- [ ] Mol File
- [ ] SMILES
- [ ] InChI String
- [x] MS-Ready SMILES
- [ ] QSAR-Ready SMILES

Intrinsic And Predicted Properties
- [x] Molecular Formula
- [ ] Average Mass
- [ ] Monoisotopic Mass
- [ ] TEST Model Predictions
- [x] OPERA Model Predictions

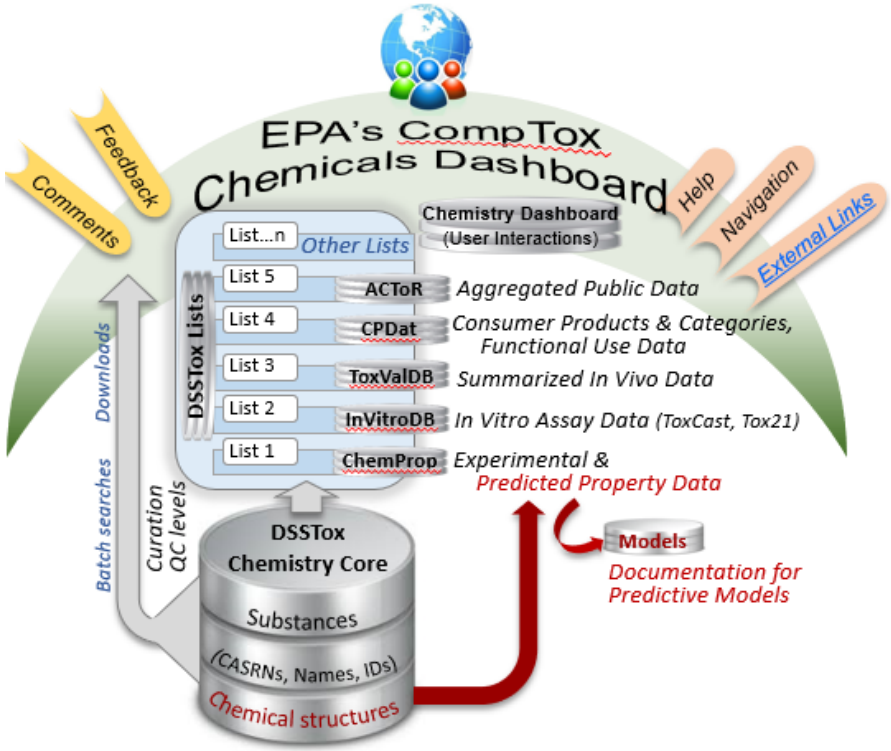
Metadata
- [ ] Curation Level Details
- [ ] NHANES/Predicted Exposure
- [ ] Data Sources
- [x] Include ToxVal Data Availability
- [x] Assay Hit Count
- [x] Number of PubMed Articles

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	INPUT	FOUND_BY	DTXSID	PREFERRE	CASRN	INCHIKEY	IUPAC_NAI	MOLECULA	TOXVAL_D	TOXCAST_	TOXCAST_	MS_READY	NUMBER_C	IRIS_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(eth	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	ClCCOCCCl	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((	4308	-	-	1.179E-10	5.05695
6	1464-53-5	CAS-RN	DTXSID00	2,2'-Bioxiran	1464-53-5	ZFIVKAOQE	2,2'-Bioxiran	C4H6O2	Y	-	-	C1OC1C1C	363	-	-	4.383E-12	1.27107
7	22224-92-6	CAS-RN	DTXSID30	Fenamiphos	22224-92-	ZCJPOPBZI	Ethyl 3-meth	C13H22NO3	Y	10.8	105/972	CCOP(=O)(	58	Y	-	1.66E-11	2.3394
8	359-06-8	CAS-RN	DTXSID40	Fluoroacetyl	359-06-8	ZBHDTYQJ	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-	O4STl2	Y	-	-	-	34	Y	Y	-	-
11	62207-76-5	CAS-RN	DTXSID40	Bis(3-fluoro	62207-76-	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 br	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-(Dimethyla	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	YLQBMQCU	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-(diethoxyn	3037-72-7	YHFFINXFN	4-[Diethoxy(	C9H23NO2S	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	S-[(5-Metho	C9H13O6PS	Y	-	-	COC1=COC	-	-	-	4.355E-11	1.18341
20	12108-13-3	CAS-RN	DTXSID90	(Methylcyclo	12108-13-	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 acetate	108-05-4	XTXRWKRV	Ethenyl 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-	XPIBKKWN	-	B5H9	Y	-	-	-	-	-	-	-	-
25	75-74-1	CAS-RN	DTXSID00	Tetramethyl	75-74-1	XOOGZRUE	Tetramethyl	C4H12Pb	Y	-	-	C[Pb](C)(C)	24	-	-	-	-

Worksheet1

Conclusion

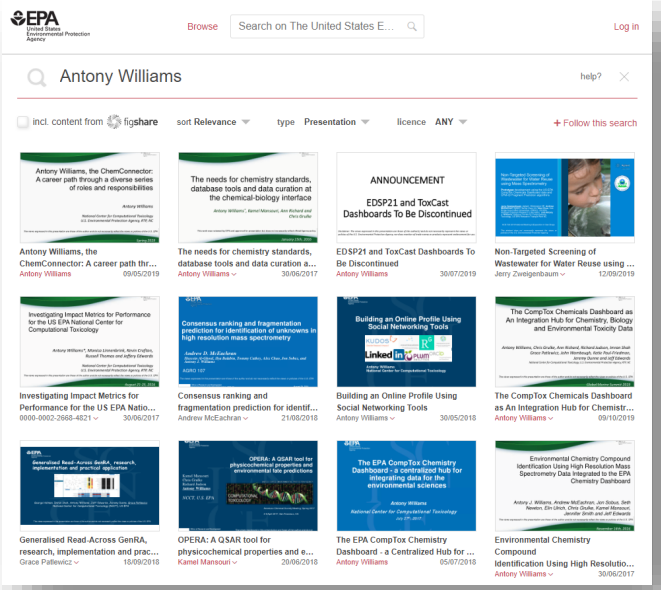
- Dashboard access to data for ~883,000 chemicals (and growing)
- Data aggregation for ALL data sources continues unabated
- Data curation is essential. Bigger does NOT mean better
- Flexible search capabilities continue to expand release-to-release but our efforts are in a rearchitecture effort

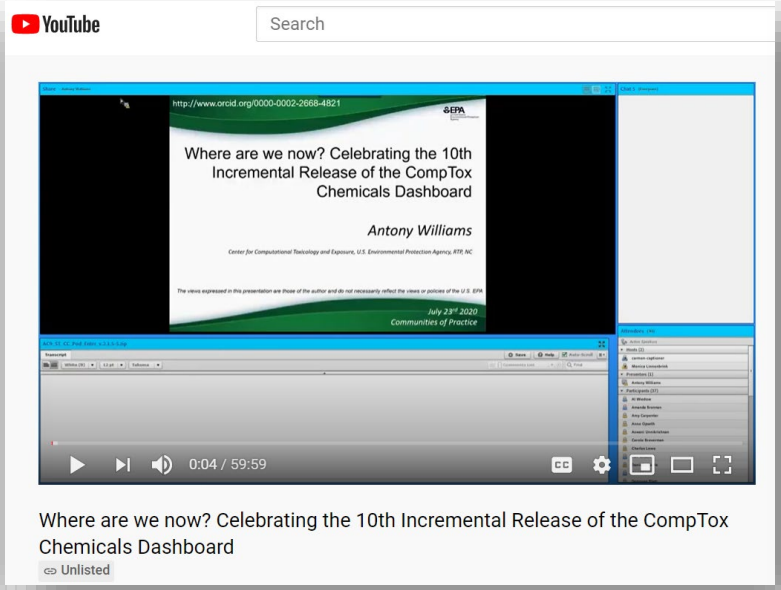


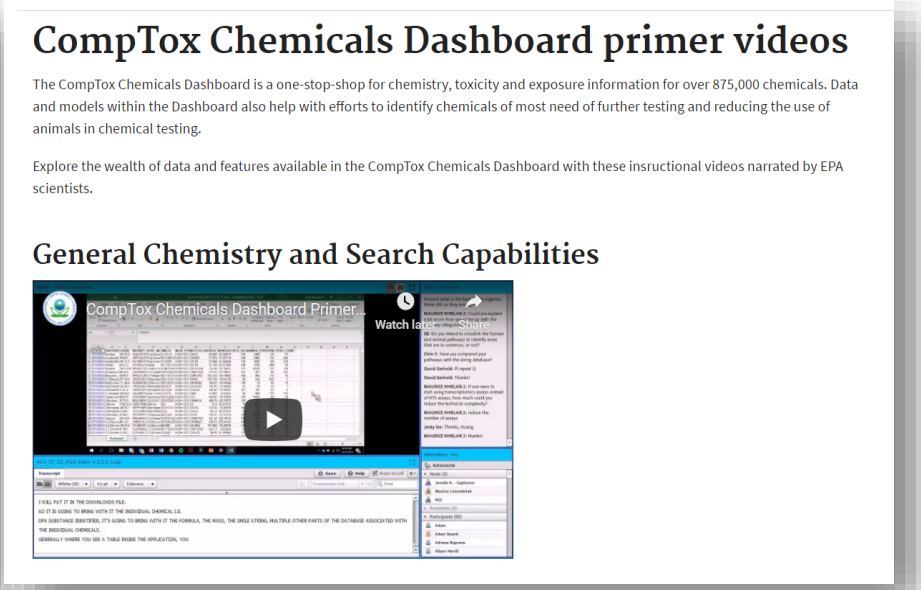
Online Materials

You want to know more…

- Lots of resources available
  - Presentations: https://tinyurl.com/w5hqs55
  - Communities of Practice Videos: https://rb.gy/qsbno1
  - Manual: https://rb.gy/4fgydc
  - Latest News: https://comptox.epa.gov/dashboard/news_info







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- Contact: Williams.Antony@epa.gov
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EPA's Center for Computational Toxicology and Exposure