



EPA Tools and Resources Webinar CompTox Chemicals Dashboard:

***Data and Tools to Support Chemical
and Environmental Risk Assessment***

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National Center for Computational Toxicology
US EPA Office of Research and Development**

September 11, 2019

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

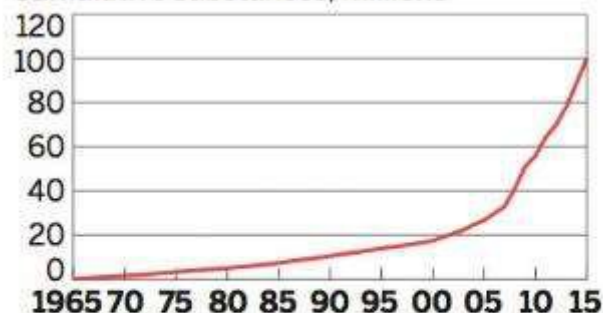
Problem: Too Many Chemicals, Too Few Resources

- Timely characterization of human and ecological risk posed by thousands of existing and emerging chemicals is a critical challenge to protect public health and the environment

Chemical & Engineering News 2015 93(32), p14

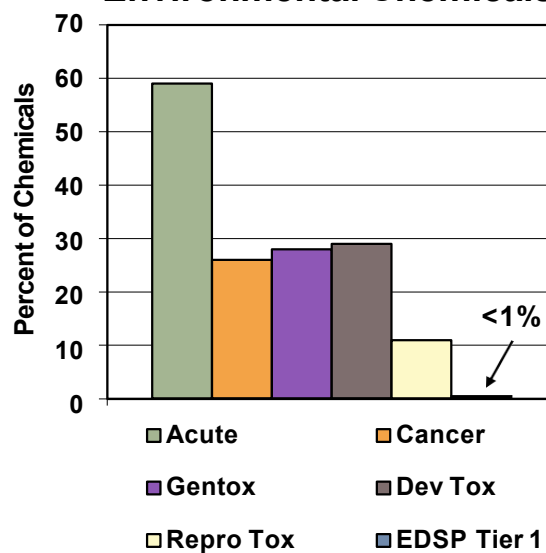
EXPONENTIAL GROWTH In the past 10 years, CAS has added 75 million entries to its registry—triple the number added during the first 40 years.

Cumulative substances, millions



SOURCE: CAS

Data for
Environmental Chemicals

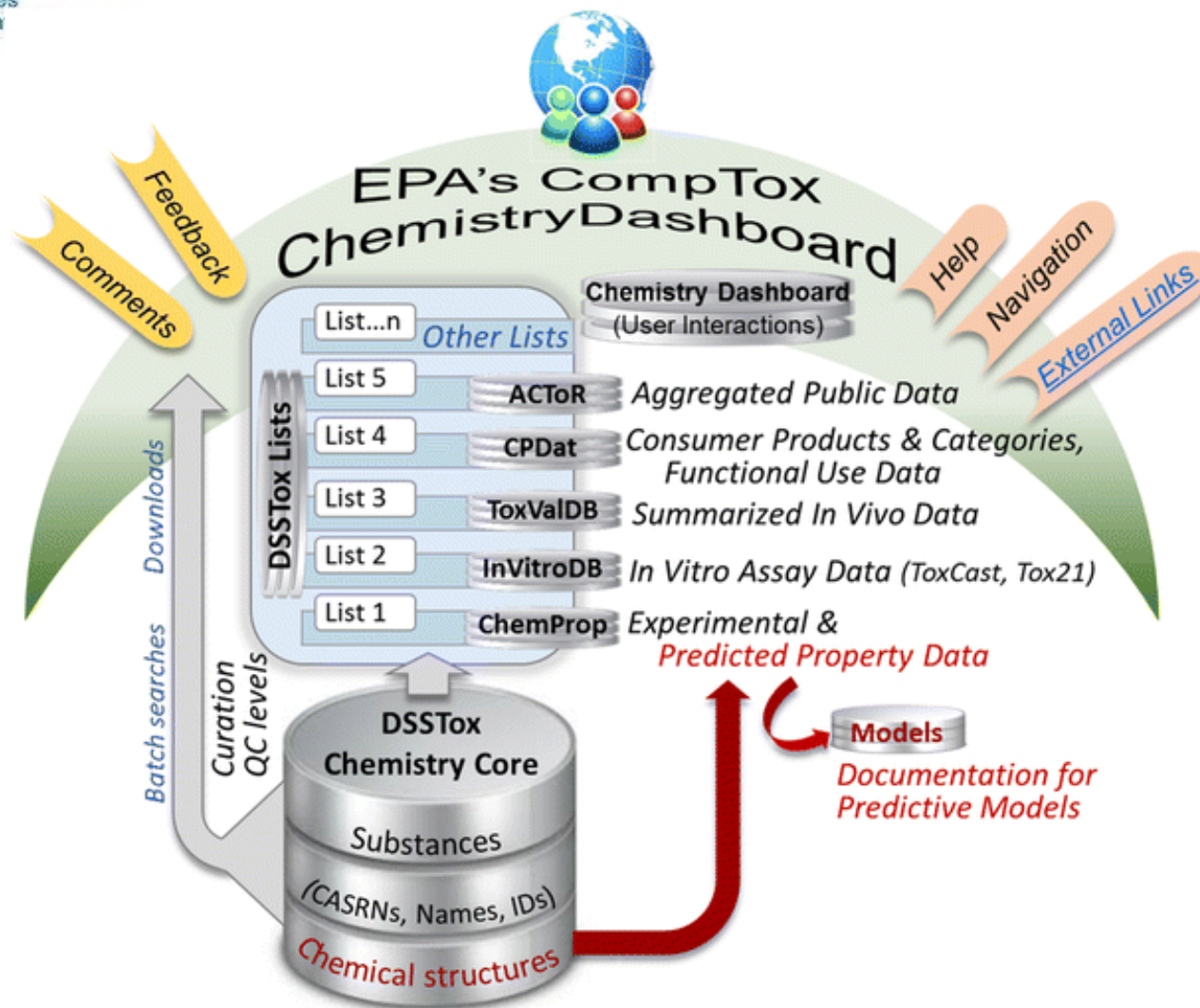


Modified from Judson *et al.*, EHP 2010

Approach

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

Approach



Williams et al. J of Cheminformatics 9: 61 (2017)

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

EPA's CompTox Chemicals Dashboard

A publicly accessible website delivering:

- ~875,000 chemicals with related property data
- Experimental and predicted physicochemical property data
- Integration to “biological assay data” for 1000’s 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
- Downloadable Open Data for reuse and repurposing
- Many features (only highlighting a few)
- Access to multiple tools (direct data interpolation and predictive) for multiple disciplines



875 Thousand Chemicals

Chemicals

Product/Use Categories

Assay/Gene

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

☐ Identifier substring search

See what people are saying, read the dashboard [comments!](#)

Cite the Dashboard Publication [click here](#)

Latest News

[Read more news](#)

August 9th 2019 - New release (3.0.9) in time for ACS Fall Meeting

August 14th, 2019 at 4:39:37 PM

A new version of the Dashboard has been released in time for the ACS Fall meeting. Included in this release are updates to data in the ToxVal database, an update to the in vitro database ([version 3.2](#)), and the release also addresses a number of minor bugs and includes a short list of additional functionality as described in the [Release Notes here](#).



Detailed Chemical Pages



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)

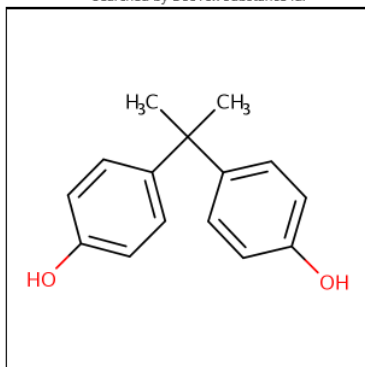
RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

COMMENTS



Wikipedia

Bisphenol A (BPA) is an organic synthetic compound with the chemical formula $(\text{CH}_3)_2\text{C}(\text{C}_6\text{H}_4\text{OH})_2$ 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](#)

Quality Control Notes

No Quality Control notes.

Intrinsic Properties

Structural Identifiers

Linked Substances

Presence in Lists

Record Information



Discover.

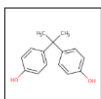
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Connect.

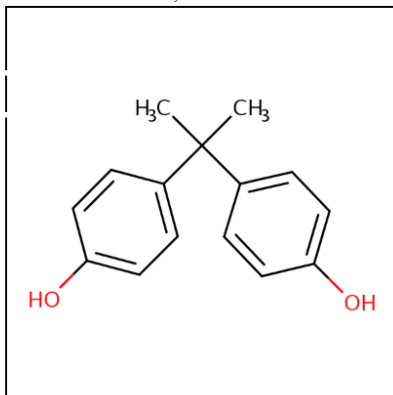
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Searched by DSSTox Substance Id.



Wikipedia

Quality Control Notes

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 September 03, 2019), 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



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Properties



Bisphenol A
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Searched by DSSTox Substance Id.

Property

Summary

Summary


Download Columns

Search query


Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
LogP: Octanol-Water	3.32 (1)	3.29		3.43	3.32	2.40 to 3.64	-
Melting Point	155 (7)	139	156	138	153 to 156	125 to 157	°C
Boiling Point	200 (1)	363		360	200	343 to 401	°C
Water Solubility	5.26e-4 (1)	9.62e-4		1.00e-3	5.26e-4	5.35e-4 to 1.31e-3	mol/L
Vapor Pressure	-	8.37e-7		3.43e-7	-	6.83e-8 to 2.59e-6	mmHg
Flash Point	-	190		190	-	188 to 192	°C
Surface Tension	-	46.0			-	46.0	dyn/cm
Index of Refraction	-	1.60			-	1.60	-
Molar Refractivity	-	68.2			-	68.2	cm ³
Polarizability	-	27.0			-	27.0	Å ³
Density	-	1.17		1.17	-	1.14 to 1.20	g/cm ³
Molar Volume	-	200			-	200	cm ³
Thermal Conductivity	-	150			-	150	mW/(m*K)
Viscosity	-	9.66			-	9.66	cP
Henry's Law	-	1.26e-7			-	1.26e-7	atm-m ³ /mole
LogKoa: Octanol-Air	-	8.38			-	8.38	-

16 records

Environmental Fate and Transport


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

Property

Summary

Download Columns

Search query

Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
Bioaccumulation Factor	-	173			-	173	-
Bioconcentration Factor	133 (93)	93.5	150	72.0	1.70 to 250	43.7 to 173	-
Soil Adsorp. Coeff. (logKoc)	-	1.34e+3		1.34e+3	-	1.24e+3 to 1.44e+3	L/kg
Atmos. Hydroxylation Rate	-	1.64e-11			-	1.64e-11	cm3/molecule*sec
Biodeg. Half-Life	-	15.1			-	15.1	days
Fish Biotrans. Half-Life (Km)	1.86 (1)	1.63			1.86	1.63	days

6 records

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

COMMENTS

Chemical Hazard Data



Bisphenol A
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EXECUTIVE SUMMARY

PROPERTIES

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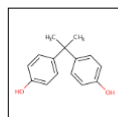
RELATED SUBSTANCES

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▶ LITERATURE

LINKS

COMMENTS



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▶ ADME

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▶ BIOACTIVITY

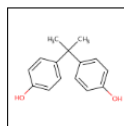
SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

▶ LITERATURE



Bisphenol A
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Searched by DSSTox Substance Id.

DataType

Screening Level

Download

Columns

Hazard

Human Eco

More	Priority	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species
	4	HBSL	Noncancer	chronic	300	ug/L	-	oral	-
	2	screening level (residential soil)	THQ = 0.1	chronic	320	mg/kg	-	-	-
	2	screening level (industrial soil)	THQ = 0.1	chronic	4100	mg/kg	-	-	-
	2	screening level (tap water)	THQ = 0.1	chronic	77	ug/L	-	-	-
	2	risk-based SSL	THQ = 0.1	chronic	5.8	mg/kg	-	-	-
	2	screening level (residential soil)	THQ = 1	chronic	3200	mg/kg	-	-	-
	2	screening level (industrial soil)	THQ = 1	chronic	41000	mg/kg	-	-	-

Sources of Exposure to Chemicals

Bisphenol A

Copy Share Submit Comment Search all data

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DETAILS

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BIOACTIVITY

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GENRA (BETA)

RELATED SUBST

SYNONYMS

ITERATI

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

PRODUCT & USE CATEGORIES

CHEMICAL WEIGHT FRACTION

CHEMICAL FUNCTIONAL USE

TOXICS RELEASE INVENTORY

MONITORING DATA

EXPOSURE PREDICTIONS

PRODUCTION VOLUME

BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

ITERATI

Bisphenol A

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Bisphenol A

80-05-7 | DTXSID7020182

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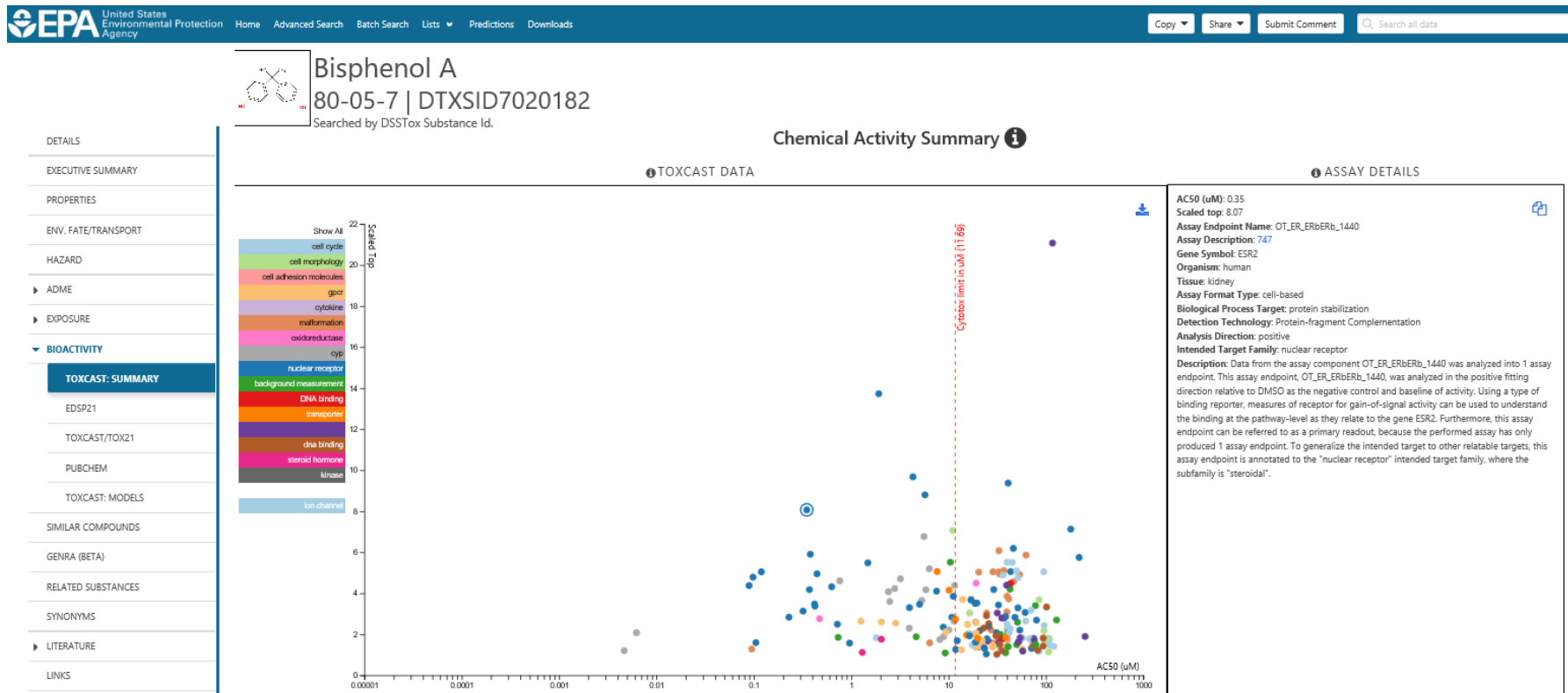
i National Health and Nutrition Examination Survey (NHANES) Inferences (mg/kg-bw/day)

Download

Demographic	Lower 95th Limit	Upper 95th Limit
Ages 6-11	3.80e-5	4.92e-5
Ages 12-19	2.55e-5	3.38e-5
Ages 20-65	2.79e-5	3.27e-5
Ages 65+	1.91e-5	2.31e-5
BMI > 30	2.38e-5	2.74e-5
BMI < 30	3.02e-5	3.30e-5
Repro. Age Females	2.83e-5	3.31e-5
Females	2.58e-5	3.03e-5
Males	2.94e-5	3.37e-5
Total	2.86e-5	3.08e-5

10 records

In Vitro Bioassay Screening ToxCast Summary



Similar Compounds



Bisphenol A
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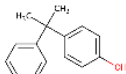

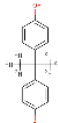
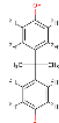
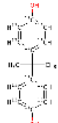
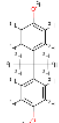
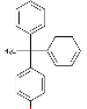
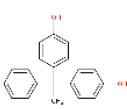
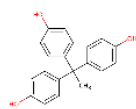
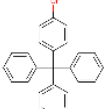
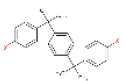
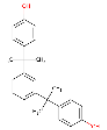
Searched with a similarity threshold of 0.8

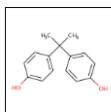
- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
- TOXCAST: SUMMARY
- EDSP21
- TOXCAST/TOX21
- PUBCHEM
- TOXCAST: MODELS
- SIMILAR COMPOUNDS**
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS

390 chemicals

Select all Download Send to Batch Search Similarity DTXSID CASRN TOXCAST Similarity

Hide chemicals that are: Filter by Name or CASRN

 <p>4-Cumylphenol DTXSID:DTXSID3022536 CASRN:599-64-4 TOXCAST:287/739 Similarity:1.00</p>	 <p>4,4'-(1,3-¹³C₆)Propane-2,2-diyldiphenol DTXSID:DTXSID30747173 CASRN:263261-64-9 TOXCAST:- Similarity:1.00</p>	 <p>4,4'-(¹³H₆)Propane-2,2-diyldiphenol DTXSID:DTXSID00584370 CASRN:86588-58-1 TOXCAST:- Similarity:1.00</p>	 <p>4,4'-(Propane-2,2-diyldi(¹³H₆))phenol DTXSID:DTXSID40662328 CASRN:92739-58-7 TOXCAST:- Similarity:1.00</p>	 <p>4,4'-(Propane-2,2-diyldi(¹³C₆))phenol DTXSID:DTXSID10675703 CASRN:263261-65-0 TOXCAST:- Similarity:1.00</p>	 <p>4,4'-(¹³H₆)Propane-2,2-diyldi(¹³H₆))phenol DTXSID:DTXSID40583721 CASRN:96210-87-6 TOXCAST:- Similarity:1.00</p>
 <p>4-(1,1-diphenylethyl)phenol DTXSID:DTXSID50288558 CASRN:6938-97-2 TOXCAST:- Similarity:1.00</p>	 <p>4,4'-(1-Phenylethylidene)bisphenol DTXSID:DTXSID5051444 CASRN:1571-75-1 TOXCAST:78/273 Similarity:1.00</p>	 <p>4,4'-Ethane-1,1,1-triyltriphenol DTXSID:DTXSID2037712 CASRN:27955-94-8 TOXCAST:242/679 Similarity:1.00</p>	 <p>4-(Triphenylmethyl)phenol DTXSID:DTXSID8075172 CASRN:978-86-9 TOXCAST:- Similarity:1.00</p>	 <p>Bisphenol P DTXSID:DTXSID0058693 CASRN:2167-51-3 TOXCAST:- Similarity:1.00</p>	 <p>Phenol, 4,4'-(1,3-phenylenebis(1-methyl-4-ethoxyphenyl)) DTXSID:DTXSID7065548 CASRN:13595-25-0 TOXCAST:- Similarity:1.00</p>



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

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EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

GOOGLE SCHOLAR

Abstract Sifter

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

Female Reproduction

Retrieve Articles ⁱ

1970 of 1970 articles loaded...

Optionally, edit the query before retrieving.

("80-05-7" OR "Bisphenol A") AND (((reproduction OR Reproductive Physiological Phenomena[mh]) AND female) OR breast OR Genitalia, Female[mh] OR OR pregnancy OR uterus or oogenesis or Ovary or Genital Diseases, Female[mh])

Update Article Counts

View / hide
queries

Heat Map
by column

Heat Map by
row

Summary heading

Preferred Name	Chemical / Entity query	Genetox	Cancer	ReproTox	NeuroTox	DevTox
TBBPA	tetrabromobisphenol A OR TBBPA	15	40	43	73	52
TPHP	triphenyl phosphate	8	10	17	23	21
TDCPP/TDCIPP	tris(1,3-dichloro-2-propyl)phosphate OR 13674-84-5 OR TDCPP	9	14	18	24	33
TCEP	Tris-2-chloroethyl phosphate OR 115-96-8	12	15	12	24	11
HBCDD	Hexabromocyclododecane	16	16	32	43	29
Melamine	Melamine	100	308	31	35	23
BDE-100	2,2',4,4',6-Pentabromodiphenyl ether OR BDE-100 OR 189084-64-8	10	26	72	81	57
HBB	hexabromobenzene	0	1	1	2	3
DBP	2,4-dibromophenol	2	1	2	0	2
Dechlorane	dechlorane	6	4	4	7	7
Organophosphate family	Organophosphates	1277	1981	725	3189	796



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80-05-7 | DTXSID7020182

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PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

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SYNONYMS

LITERATURE




















LINKS

COMMENTS


















General

-  EPA Substance Registry Service
-  Household Products Database
-  PubChem
-  ChempSpider
-  CPCat
-  DrugBank
-  Wikipedia
-  MSDS Lookup
-  ChEMBL
-  Chemical Vendors
-  ToxPlanet
-  ACS Reagent Chemicals
-  ChemHat: Hazards and Alternatives Toolbox
-  Wolfram Alpha
-  ECHA Infocard
-  ChemAgora
-  ChEBI
-  NIST Chemistry Webbook
-  Wikidata
-  WEBWISER
-  PubChem Safety Sheet
-  NIOSH Chemical Safety Cards
-  ECHA Brief Profile
-  Consumer Product Information Database
-  HMDB
-  CalEPA OEHHA
-  Sigma-Aldrich Chemicals











Toxicology

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





Publications

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

Analytical

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

Prediction

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

Searching for more than one Chemical: Batch Searching

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

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

Select Output Format:

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

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

bisphenol a
phthalate

Presence in Lists:

☐ Pharmaceuticals from ZINC15

☐ 40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities

☐ AEGLS: Acute Exposure Guideline Levels

☐ Amphibole Minerals

☐ ANDROGEN: Androgen Receptor Chemicals

☐ ARTICLE: Bench-Mark Dose Human Health Assessment List (Wignall et al., 2014)

☐ ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (CERAPP)

☐ ATSDR: Minimal Risk Levels (MRLs) for Hazardous Substances

☐ ATSDR: Toxic Substances Portal Chemical List

☐ CalEPA Office of Environmental Health Hazard Assessment

☐ Chemicals in human blood (plasma and serum)

☐ DRUGS: DrugBank database from the University of Alberta

☐ DRUGS: Statin drugs

☐ DRUGSINORMAN: ITNANTIBIOTIC list of antibiotics

☐ DRUGSINORMAN: Pharmaceutical List with EU, Swiss, US Consumption Data

☐ DRUGSINORMAN: Target Pharmaceutical/Drug List from University of Athens

☐ DRUGSWIKILIST: Veterinary Drugs

☐ EPA Drinking Water Treatability Database

Select List

Select List

EPA|TSCA: List of Chemicals Undergoing Prioritization: High Priority Candidates

Search TSCA|HIGHPRI Chemicals

☐ Identifier substring search

List Details

Description: On March 20, 2019, EPA released a list of 40 chemicals to begin the prioritization process. TSCA requires EPA to publish this list of chemicals to begin the prioritization process and designate 20 chemicals as "high-priority" for subsequent risk evaluation and to designate 20 chemicals as "low-priority," meaning that risk evaluation is not warranted at this time. Publication in the Federal Register activates a statutory requirement for EPA to complete the prioritization process in the next nine to twelve months, allowing EPA to designate 20 chemicals as high priority and 20 chemicals as low priority by December 2019. The chemicals in the list below are the 20 high priority candidates.

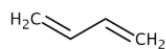
Number of Chemicals: 20

Select all Download Send to Batch Search Default 20 chemicals

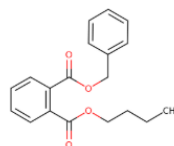
DTXSID TOXCAST CASRN

Hide chemicals that are:

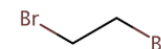
Filter by Name or CASRN



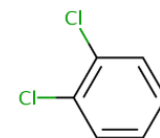
1,3-Butadiene
DTXSID:DTXSID3020203
TOXCAST:-
CASRN:106-99-0



Benzyl butyl phthalate
DTXSID:DTXSID3020205
TOXCAST:71/719
CASRN:85-68-7



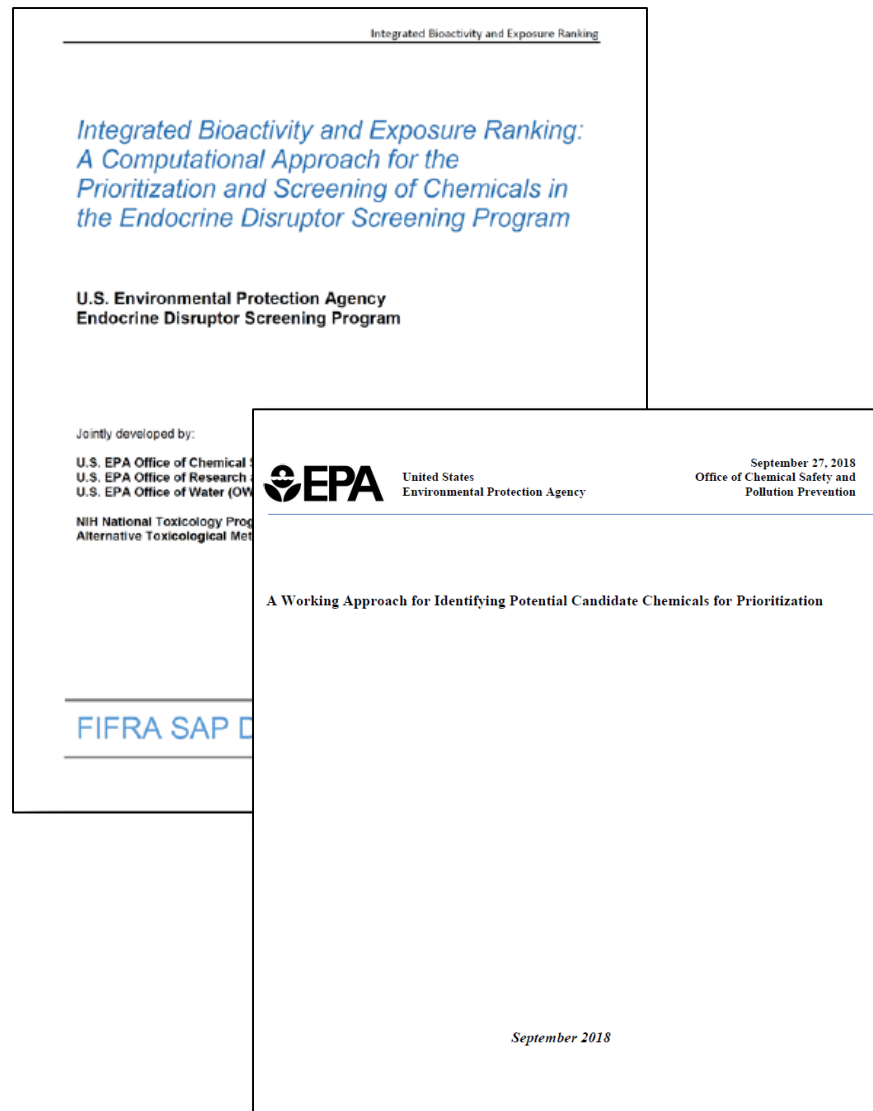
1,2-Dibromoethane
DTXSID:DTXSID3020415
TOXCAST:13/604
CASRN:106-93-4



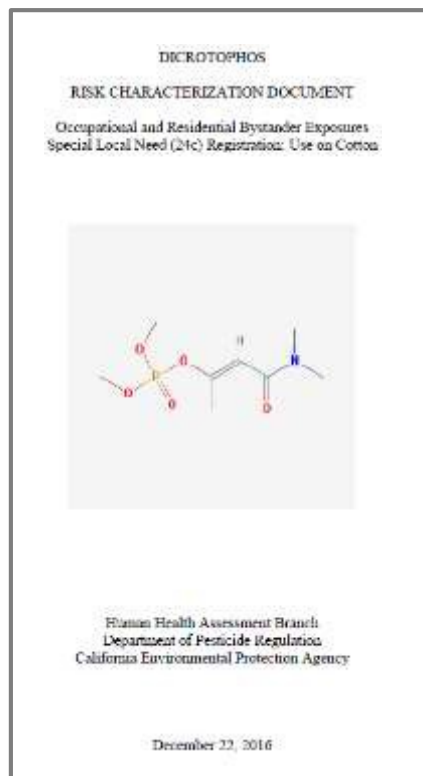
1,2-Dichlorobenzene
DTXSID:DTXSID6020430
TOXCAST:12/675
CASRN:95-50-1

Impact

- CompTox Chemicals Dashboard integrates chemical data
- Used by EPA and others to support chemical assessment
 - Endocrine Disruptor Screening Program in the 21st Century (EDSP21)
 - Screening and Prioritization in support of TSCA



CalEPA Pesticide Assessments



Dicrotophos RCD for Cotton Use	
December 22, 2016	
Table of Contents	
CONTRIBUTORS AND ACKNOWLEDGMENTS	ii
Table of Contents	iii
List of Tables	iv
SUMMARY	vii
I. INTRODUCTION	1
I.A. ENVIRONMENTAL FATE	1
I.A.1. Air	1
I.A.2. Soil	1
I.A.3. Water	2
II. HAZARD IDENTIFICATION	3
II.A. Pharmacokinetics	3
II.B. Neurotoxicity	4
II.B.1. Acute Neurotoxicity Study in Rats	4
II.B.2. Comparative Cholinesterase Studies in Rats	5
II.B.3. 14-Day Oral Exposure to Pre-weaning and Young Adults	7
II.B.4. 28-Day Tissue Toxicity in Adult Rats	7
II.B.5. 28-Day Subacute Exposure to Adult Rats	8
II.B.6. Subchronic Neurotoxicity Study in Adult Rats	9
II.B.7. Developmental Neurotoxicity Study in Rats	9
II.B.8. Rat Chronic Toxicity/Reproductive Study	12
II.B.9. Toxicokinetic Study of Cholinesterase Inhibition	13
II.C. Weight of Evidence for Chronicity	17
II.C.1. Mouse Oncogenicity Study	17
II.C.2. Rat Chronic Chronic Toxicity/Reproductive Study	18
II.C.3. Genotoxicity	18
II.C.4. Structure-Activity Relationships	20
II.C.5. Toxicity Data	20
II.C.6. Conclusions	21
II.D. Critical Endpoints and Reference Levels	25
III. EXPOSURE ASSESSMENT	25
III.A. Dietary and Drinking Water Exposure	25
III.A.1. Residential Data	25
III.A.2. Sources	26

“California benefits significantly from our partnership with EPA ORD. We use ToxCast data to provide valuable insight into how chemicals may cause toxicity, and we use their lifecycle analytic and exposure modeling and monitoring for various state efforts including our work on safer consumer products. EPA ORD resources are helping us to make more informed decisions about the potential health effects of chemicals.”

– **CalEPA Secretary Matthew Rodriquez**

- ToxCast data used for weight of evidence decisions regarding health effects for pesticides

Impact

Pharmaceuticals and Chemicals of Concern in Rivers: Occurrence and Biological Effects



 Minnesota Pollution Control Agency

January 2017

“EPA’s variety of tools have been critical in developing aquatic toxicity profiles (ATPs) for contaminants detected across Minnesota. The MPCA uses EPA’s estimation tools and databases to quickly obtain relevant information about contaminants that have only recently been detected in an aquatic environment. Prior to the development of these tools, information about contaminants has been limited or time-consuming to find. The profiles combine contaminant information such as fate in the environment, aquatic life toxicity, and endocrine activity to screen contaminants detected in Minnesota. The MPCA uses this information to communicate potential effects of the contaminants found in Minnesota and to identify pollution prevention opportunities for contaminants of highest concern.”

– ***MPCA Commissioner John Linc Stine***

Conclusion

- EPA's CompTox Chemicals Dashboard provides access to data for ~875,000 chemicals
- Dashboard is an integration hub for multiple “modules” and tools to support multiple environmental applications
- Data releases twice a year (at present) and supported with ongoing manual curation efforts
- Updates released in both March and August 2019
 - New bioassay data in the InvitroDBv3.1 release
 - New toxicity data added - ~800,000 toxicity data points
 - Focused data efforts for PFAS chemical lists and properties



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