



EPA Tools and Resources Webinar

CompTox Chemicals Dashboard: *Data and Tools to Support Chemical and Environmental Risk Assessment*

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US EPA Office of Research and Development

September 11, 2019

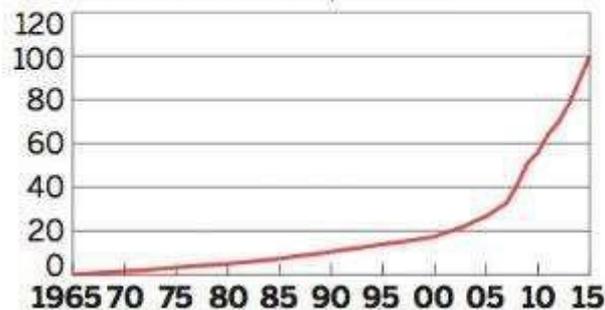
Problem: Too Many Chemicals, Too Few Resources

- 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.

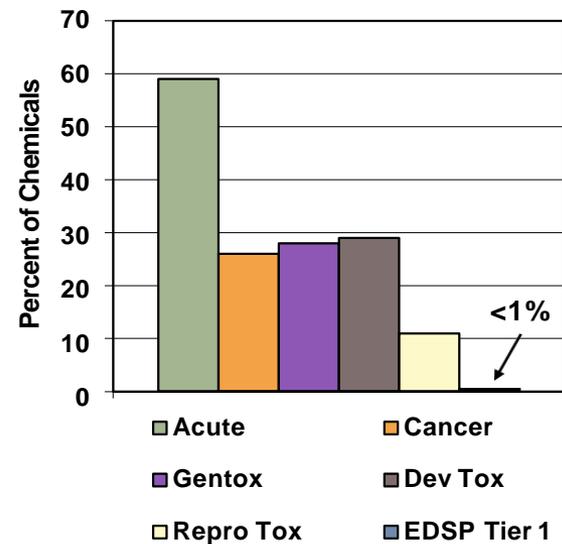
Cumulative substances, millions



SOURCE: CAS

*CAS – Chemical Abstracts Service

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**

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](#).





Bisphenol A
80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

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ENV. FATE/TRANSPORT

HAZARD

▶ ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

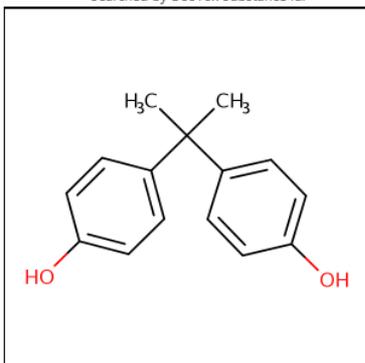
RELATED SUBSTANCES

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.

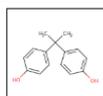
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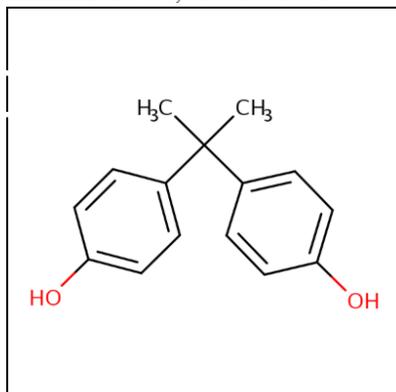
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Wikipedia

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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



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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 ² 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

Properties, Environmental Fate and Transport



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- GENRA (BETA)
- RELATED SUBSTANCES
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- ▶ LITERATURE
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Summary

Download Columns

Summary

Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range
Bioaccumulation Factor	-	173			-	173
Bioconcentration Factor	133 (93)	93.5	150	72.0	1.70 to 250	43.7 to 1000
Soil Adsorp. Coeff. (logKoc)	-	1.34e+3		1.34e+3	-	1.24e+3 to 1.34e+3
Atmos. Hydroxylation Rate	-	1.64e-11			-	1.64e-11
Biodeg. Half-Life	-	15.1			-	15.1
Fish Biotrans. Half-Life (Km)	1.86 (1)	1.63			1.86	1.63

6 records



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Hazard

Data Type

Toxicity Value

Download Columns

Human Eco

Search query

More	Priority	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	7	MEG	Short-term Critical Air	short-term	500	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Marginal Air	short-term	100	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Negligible Air	short-term	15	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Soil Negligible Soil	chronic	106000	mg/kg	-	soil	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Long-Term, 5L/d Negligible Water	chronic	7	mg/L	-	oral	-	TG 230 Military Exposure Guidelines Table	DOD
	6	RID	-	chronic	0.05	mg/kg-day	-	oral	rat	Wignall	Wignall
	5	RID	-	chronic	0.05	mg/kg-day	-	-	-	MSC Table 5	Pennsylvania DEP Tox/Values
	4	RID	-	chronic	0.05	mg/kg-day	chronic	oral	rat	IRIS	Chiu
	3	RID	Reference Dose for Subchronic Oral Exposure (SRD)	chronic	0.6	mg/kg-day	-	oral	rat	EPA/ORNL/OLEM	HEAST
	1	RID	-	chronic	0.05	mg/kg-day	-	oral	-	EPA NCEA	IRIS

10 records



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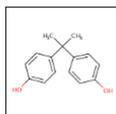
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Data Type

Point of Departure

Download Columns 10

Hazard

Hazard

Human Eco

Search query

More	Priority	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	7	LOAEL	Repeated dose toxicity; oral	subacute	600	mg/kg-day	subacute	oral	rat	eChemPortal	ECHA
	7	NOEL	Repeated dose toxicity; oral	multigenerational reproductive	30	ppm	multigeneration	oral	mouse	eChemPortal	ECHA
	7	NOAEL	Repeated dose toxicity; oral	multigenerational reproductive	300	ppm	multigeneration	oral	mouse	eChemPortal	ECHA
	7	NOAEL	Repeated dose toxicity; oral	multigenerational reproductive	300	ppm	multigeneration	oral	mouse	eChemPortal	ECHA
	7	NOEL	Repeated dose toxicity; oral	multigenerational reproductive	75	ppm	multigeneration	oral	rat	eChemPortal	ECHA
	7	NOAEL	Repeated dose toxicity; oral	multigenerational reproductive	750	ppm	multigeneration	oral	rat	eChemPortal	ECHA
	7	NOAEL	Repeated dose toxicity; oral	multigenerational reproductive	750	ppm	multigeneration	oral	rat	eChemPortal	ECHA
	7	NOEL	-	repeat dose	40	mg/kg-day	repeat dose	oral	rat	Japan NITE	HESS



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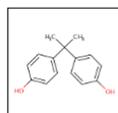
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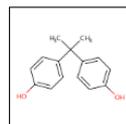
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Data Type

Screening Level

Download Columns

Hazard

Human Eco

More	Priority	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Spe
	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	-	-	-



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Product and Use Categories (PUCs) i

Download Columns 10

Search query

Product or Use Categorization	Categorization type	Number of Unique Products
adhesive	CPat Cassette	17
manufacturing, metals	CPat Cassette	17
paint	CPat Cassette	16
manufacturing, machines	CPat Cassette	12
manufacturing, plastics	CPat Cassette	11
building_material, flooring	CPat Cassette	8
construction	CPat Cassette	8
surface_treatment, metals	CPat Cassette	8
stabilizer	CPat Cassette	7
building_construction	CPat Cassette	6

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

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Print Page

Toxics Release Inventory

2015 TRI Factsheet: Chemical - 4,4'-ISOPROPYLIDENEDIPHENOL, 000080057

Data Source: 2017 Updated Dataset (released April 2019)

The [Toxics Release Inventory \(TRI\)](#) tracks the management of certain toxic chemicals that may pose a threat to human health and the environment. Certain industrial facilities in the U.S. must report annually how much of each chemical is recycled, combusted for energy recovery, treated for destruction, and disposed of or otherwise released on- and off-site. This information is collectively referred to as production-related waste managed.

Map of TRI Facilities Reporting 4,4'-ISOPROPYLIDENEDIPHENOL



4,4'-ISOPROPYLIDENEDIPHENOL ranks 67 out of 499 chemicals reported to TRI in 2015 (Rank 1 = highest releases)

Under the Pollution Prevention Act of 1990, TRI collects information to track industry progress in reducing waste generation and moving towards safer waste management alternatives. EPA encourages facilities to first eliminate waste at its source (source reduction). For waste that is generated, the preferred management method is recycling, followed by energy recovery, treatment, and as a last resort, disposing of or otherwise releasing the waste. Learn more about [Pollution Prevention and TRI](#).

Quick Facts for 2015

	Chemical	United States
Number of TRI Facilities:	120	22,241
Total Production-Related Waste Managed:	15.8 million lbs	27.4 billion lbs
Total On-site and Off-site Disposal or Other Releases:	2.5 million lbs	3.4 billion lbs
Total On-site:	39.4 thousand lbs	2.9 billion lbs
• Air:	28.7 thousand lbs	688.9 million lbs
• Water:	4.4 thousand lbs	198.9 million lbs
• Land:	6.2 thousand lbs	2.0 billion lbs
Total Off-site:	2.5 million lbs	505.3 million lbs

Production-related waste managed

Sources of Exposure to Chemicals

Bisphenol A

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

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

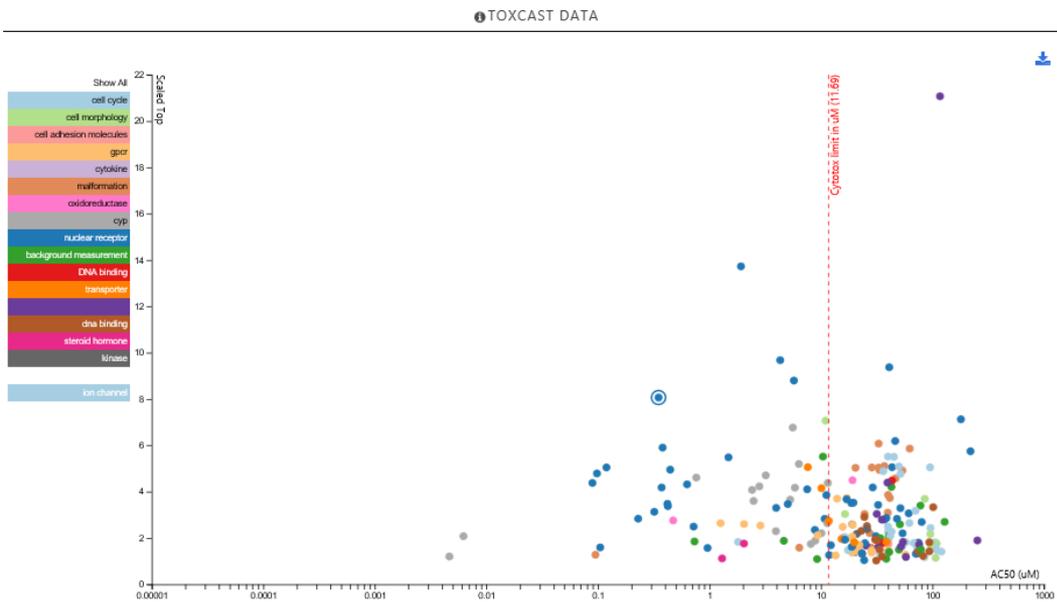
In Vitro Bioassay Screening ToxCast Summary



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 - TOXCAST: MODELS
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Chemical Activity Summary i



ASSAY DETAILS

AC50 (uM): 0.35
 Scaled top: 8.07
 Assay Endpoint Name: OT_ER_ERbERb_1440
 Assay Description: 747
 Gene Symbol: ESR2
 Organism: human
 Tissue: kidney
 Assay Format Type: cell-based
 Biological Process Target: protein stabilization
 Detection Technology: Protein-fragment Complementation
 Analysis Direction: positive
 Intended Target Family: nuclear receptor
 Description: Data from the assay component OT_ER_ERbERb_1440 was analyzed into 1 assay endpoint. This assay endpoint, OT_ER_ERbERb_1440, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of binding reporter, measures of receptor for gain-of-signal activity can be used to understand the binding at the pathway-level as they relate to the gene ESR2. 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 reliable targets, this assay endpoint is annotated to the "nuclear receptor" intended target family, where the subfamily is "steroidal".

Similar Compounds



Bisphenol A

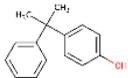
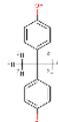
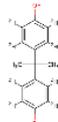
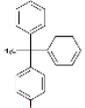
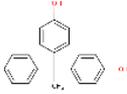
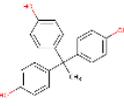
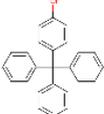
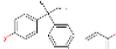
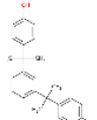
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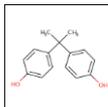
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Searched with a similarity threshold of 0.8

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 - TOXCAST: SUMMARY
 - EDSP21
 - TOXCAST/TOX21
 - PUBCHEM
 - TOXCAST: MODELS
 - SIMILAR COMPOUNDS**
 - GENRA (BETA)
 - RELATED SUBSTANCES
 - SYNONYMS
 - ▶ LITERATURE
 - LINKS

Select all Download Send to Batch Search Similarity 0 DTXSID CASRN TOXCAST Similarity 390 chemicals 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-diy(l)diphenol DTXSID:DTXSID30747173 CASRN:263261-64-9 TOXCAST:- Similarity:1.00</p>	 <p>4,4'-([²H₆]Propane-2,2-diy(l)diphenol DTXSID:DTXSID00584370 CASRN:86588-58-1 TOXCAST:- Similarity:1.00</p>	 <p>4,4'-[Propane-2,2-diy(l)d(¹³C₆)]phenol DTXSID:DTXSID40662328 CASRN:92739-58-7 TOXCAST:- Similarity:1.00</p>	 <p>4,4'-[Propane-2,2-diy(l)d(¹³C₆)]phenol DTXSID:DTXSID10675703 CASRN:263261-65-0 TOXCAST:- Similarity:1.00</p>	 <p>4,4'-([²H₆]Propane-2,2-diy(l)d(¹³C₆)]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',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...] DTXSID:DTXSID7065548 CASRN:13595-25-0 TOXCAST:- Similarity:1.00</p>



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

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.

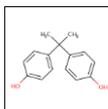
("80-05-7" OR "Bisphenol A") AND (((reproduction OR Reproductive Physiological Phenomena[mh]) AND female) OR breast OR Genitalia, Female[mh] OR OR pregnancy OR uterus or oogenesis or Ovary or Genital Diseases, Female[mh])

To find articles quickly, enter terms to sift abstracts. **i**

Download / Send to...

Download Sifter for Excel **i**

<input type="checkbox"/>	PMID	Year	Title	Authors	Journal	Rev
<input type="checkbox"/>	31471387	2019	Bisphenol A: A Concise Review of Literature and a Discussion of Health and Regulatory ...	Wazir, Mokbel	In vivo (Athens, Greece)	✓
<input type="checkbox"/>	31470855	2019	Association of urinary concentrations of early pregnancy phthalate metabolites and bisp...	Chin, Jukic, Wilcox, Weinberg, Ferguson, Calafat, ...	Environmental health : a global access science sou...	
<input type="checkbox"/>	31468552	2019	Association between peri-conceptual bisphenol A exposure in women and men and ti...	Yeum, Ju, Cox, Zhang, Stanford, Porucznik	Paediatric and perinatal epidemiology	
<input type="checkbox"/>	31455712	2019	Early Life Exposure in Mexico to ENvironmental Toxicants (ELEMENT) Project.	Perng, Tamayo-Ortiz, Tang, Sánchez, Cantoral, Me...	BMJ open	
<input type="checkbox"/>	31424210	2019	Phthalate and BPA Exposure in Women and Newborns through Personal Care Product ...	Fisher, Arbuckle, MacPherson, Braun, Feeley, Gau...	Environmental science & technology	
<input type="checkbox"/>	31393043	2019	Differences between male and female prostates in terms of physiology, sensitivity to che...	Sanches; Carvalho, Maldarine, Biancardi, Santos, ...	Cell biology international	✓
<input type="checkbox"/>	31374317	2019	Bisphenol A affects estradiol metabolism by targeting CYP1A1 and CYP19A1 in human ...	Xu, Zhang, Ye, Li	Toxicology in vitro : an international journal publishe...	
<input type="checkbox"/>	31373935	2019	An Empirical Validation of the Within-subject Biospecimens Pooling Approach to Minimiz...	Vernet, Philippat, Agier, Calafat, Ye, Lyon-Caen; Ha...	Epidemiology (Cambridge, Mass.)	
<input type="checkbox"/>	31362658	2019	Neuro-toxic and reproductive effects of BPA.	Santoro; Chianese; Troisi; Richards; Nori; Fasano; ...	Current neuropharmacology	
<input type="checkbox"/>	31362131	2019	Bisphenol A and bisphenol S exposures during pregnancy and gestational age - A longit...	Huang, Li, Xu, Zhao, Li, Zhou, Fang, Liao, Cai, Xia	Chemosphere	
<input type="checkbox"/>	31357276	2019	Development and validation of an LC-MS/MS method for the simultaneous determinatio...	Venisse; Cambien; Robin; Rouillon; Nadeau, Charle...	Talanta	



Bisphenol A

80-05-7 | DTXSID7020182

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RELATED SUBSTANCES

SYNONYMS

LITERATURE

GOOGLE SCHOLAR

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

Abstract Sifter

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



Bisphenol A

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SYNONYMS

LITERATURE

LINKS

COMMENTS

General

- EPA Substance Registry Service
- Household Products Database
- PubChem
- Chemspider
- 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
- ChemPortal
- 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
- mszCloud
- 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 Four: Select Data Output Format and Choose Data Fields to Download

Please enter one identifier per line

Enter Identifiers to Search (searches should be limited to <5000 Identifiers)
 bisphenol a
 phthalate

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:

Excel

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

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
- DRUGSINORMAN: Veterinary Drugs
- EPA Drinking Water Treatability Database

Select List

Download

Columns

10

Search query

Copy page URL

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
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	54	A list of Algal Toxins of potential interest
AMINOACIDS	LIST: Amino Acids	2019-03-05	20	Amino acids are organic compounds containing amine (-NH ₂) and carboxyl (-COOH) functional groups, along with a side chain (R group) specific to each amino acid.
AMPHIBOLES	Amphibole Minerals	2019-03-26	4	Amphiboles are an important group of inosilicate minerals.
ANTIBIOTICS	LIST: Antibiotics	2019-06-01	170	List of antibiotics and related compounds
ARCHEMICALS	ANDROGEN: Androgen Receptor Chemicals	2018-11-16	110	The list of chemicals used to identify references with in vitro AR binding . From Kleinstreuer et al http://pubs.acs.org/doi/abs/10.1021/acs.chemrestox.6b00347
ATHENSSUS	WATER: Univ. Athens Surfactant and Suspect List	2017-07-14	60	ATHENSSUS is a compilation of suspects, predicted transformation products and surfactants screened in wastewater by University of Athens, as described in Gago-Ferrero et al 2015, DOI: 10.1021/acs.est.5b03454
ATSDRLST	ATSDR: Toxic Substances Portal Chemical List	2017-03-11	200	The Agency for Toxic Substances and Disease Registry (ATSDR) is a federal public health agency of the U.S. Department of Health and Human Services.

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

Showing 1 to 10 of 196 records

Select List

Select List

Download Columns 10

PFAS

Copy Filter

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 query representations.
EPAPFASDW	PFAS[EPA: New EPA Method Drinking Water]	2019-04-17	26	EPA is developing and validating a new method for detecting these PFAS in drinking water sources.
EPAPFASDW537	PFAS[EPA]WATER: Existing EPA DW Method 537.1	2019-05-19	19	EPA has recently revised method 537.1 for the PFAS on this list to detect them in drinking water.
EPAPFASDWTREAT	PFAS[EPA]WATER: Drinking Water Treatment Technology	2019-05-19	9	EPA is gathering and evaluating treatment effectiveness and cost data for removing these PFAS from drinking water sources.
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.
EPAPFASINVIVO	PFAS[EPA: In Vivo Studies Available]	2019-04-17	23	These PFAS have published animal toxicity studies available in the online HERO database.
EPAPFASLITSEARCH	PFAS[EPA: Literature Search Completed:]	2019-04-17	23	A literature review of published toxicity studies for these PFAS

<< < 1 2 3 > >>

Showing 1 to 10 of 21 records

Select List

Select List

Download Columns 10

PFAS

Copy Filter

List Acronym	List Name
EPAPFAS75S1	PFAS[EPA:
EPAPFAS75S2	PFAS[EPA:
EPAPFASCAT	PFAS[EPA:
EPAPFASDW	PFAS[EPA: Water
EPAPFASDW537	PFAS[EPA] Method 53
EPAPFASDWTREAT	PFAS[EPA] Treatment
EPAPFASINSOL	PFAS[EPA: DMSO
EPAPFASINV	PFAS[EPA:
EPAPFASINVIVO	PFAS[EPA:
EPAPFASLITSEARCH	PFAS[EPA:

Select all

Download

Send to Batch Search

Default

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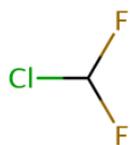
6330 chemicals

DTXSID

TOXCAST

CASRN

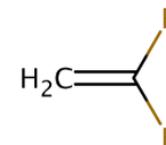
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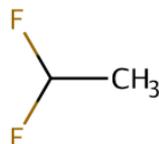
Chlorodifluoromethane
DTXSID:DTXSID6020301
TOXCAST:-
CASRN:75-45-6



Tetrafluoroethylene
DTXSID:DTXSID6021325
TOXCAST:-
CASRN:116-14-3



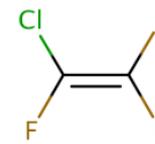
Vinylidene fluoride
DTXSID:DTXSID3021439
TOXCAST:-
CASRN:75-38-7



1,1-Difluoroethane



Perfluoropropane

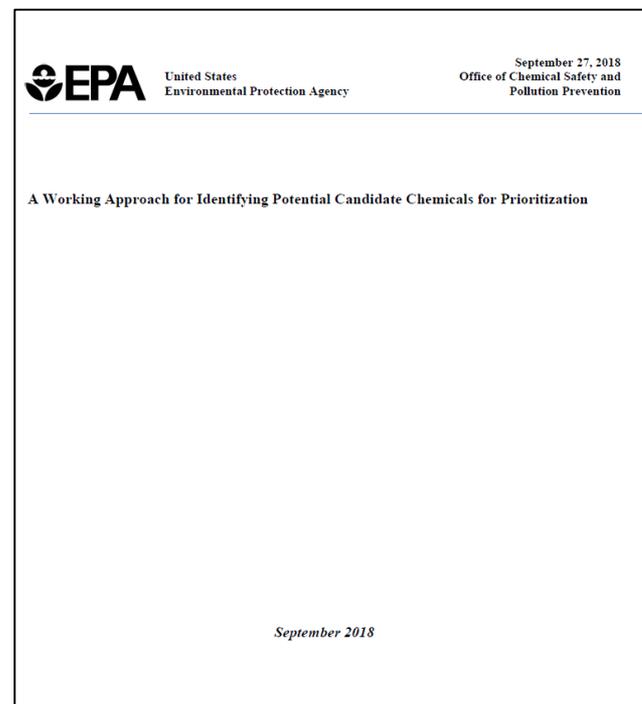


Chlorotrifluoroethylene

Impact

- **Challenge:** Need to identify a subset of both data rich and data poor compounds as possible candidates for prioritization under Toxic Substances Control Act (TSCA).
- **Solution:** CompTox Chemicals Dashboard integrates chemical data including human and ecological hazard, exposure and chemical properties that can be used to inform chemical screening and assessment.
- **Example:** TSCA's Working Approach for Identifying Potential Candidate Chemicals for Prioritization **proposed tiered decision workflows for scientific domains of interest as part of a longer-term risk-based approach for managing the larger TSCA chemical landscape.**

Example: TSCA's Working Approach for Identifying Potential Candidate Chemicals for Prioritization



Impact: Evaluating chemicals for health effects in California

Challenge: Need to make informed decisions about the potential health effects of chemicals, and determine safer and more sustainable uses of chemicals found in products that consumers buy and use.

Solution: ORD researchers provided CalEPA staff training on the use and interpretation of chemical testing data in the CompTox Chemicals Dashboard.

CalEPA uses ToxCast data to:

- Provide insight into how chemicals cause toxicity
- Perform various state efforts using the lifecycle analytic and exposure modeling and monitoring

Example: CalEPA Pesticide Assessments

DICROTOPHOS	
RISK CHARACTERIZATION DOCUMENT	
Occupational and Residential bystander Exposures Special Local Need (21c) Registration: Use on Cotton	
	
Human Health Assessment Branch Department of Pesticide Regulation California Environmental Protection Agency	
December 22, 2016	
December RCD for Cotton 21c	December 22, 2016
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- ToxCast data used for weight of evidence decisions regarding health effects for pesticides

Potential Impact: Evaluating risk of aquatic contaminants in Minnesota

Challenge: Characterizing potential effects for a wide variety of contaminants which there exists limited information.

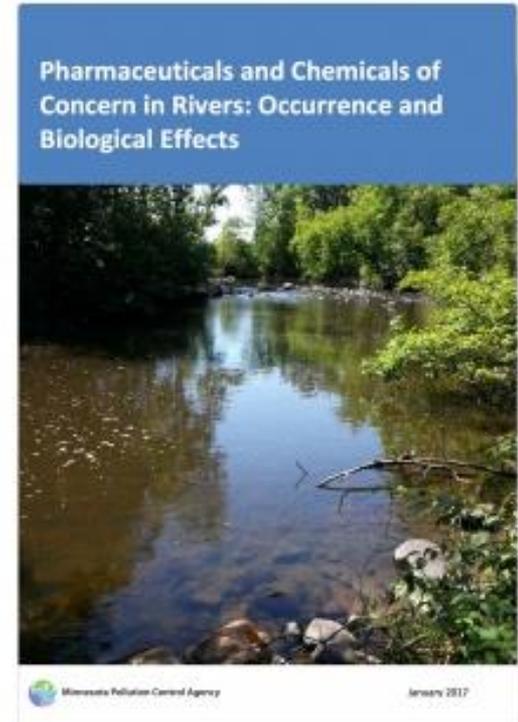
Solution: The Minnesota Pollution Control Agency (MPCA) used a suite of EPA tools, including those available under the CompTox Chemicals Dashboard, to prioritize chemicals based on toxicity effects and hazard characterization.

- Estimation Programs Interface (EPI) Suite
- ECOTOX
- Web-ICE

Using these tools, MPCA develops toxicity profiles to:

- Screen contaminants that have been detected in the state
- Monitor chemicals and prevent pollution
- Communicate the potential hazards associated with individual contaminants

Example: MPCA used tools available on the CompTox Chemicals Dashboard to identify triclocarban, an antibacterial agent commonly in soaps and lotions, as a high priority contaminant for monitoring in systems with effluent input.



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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