

EPA CompTox Chemistry Dashboard – an online resource for environmental chemists

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*National Center for Computational Toxicology
U.S. Environmental Protection Agency, RTP, NC*

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

*April 2017
ACS Spring Meeting, San Francisco, CA*

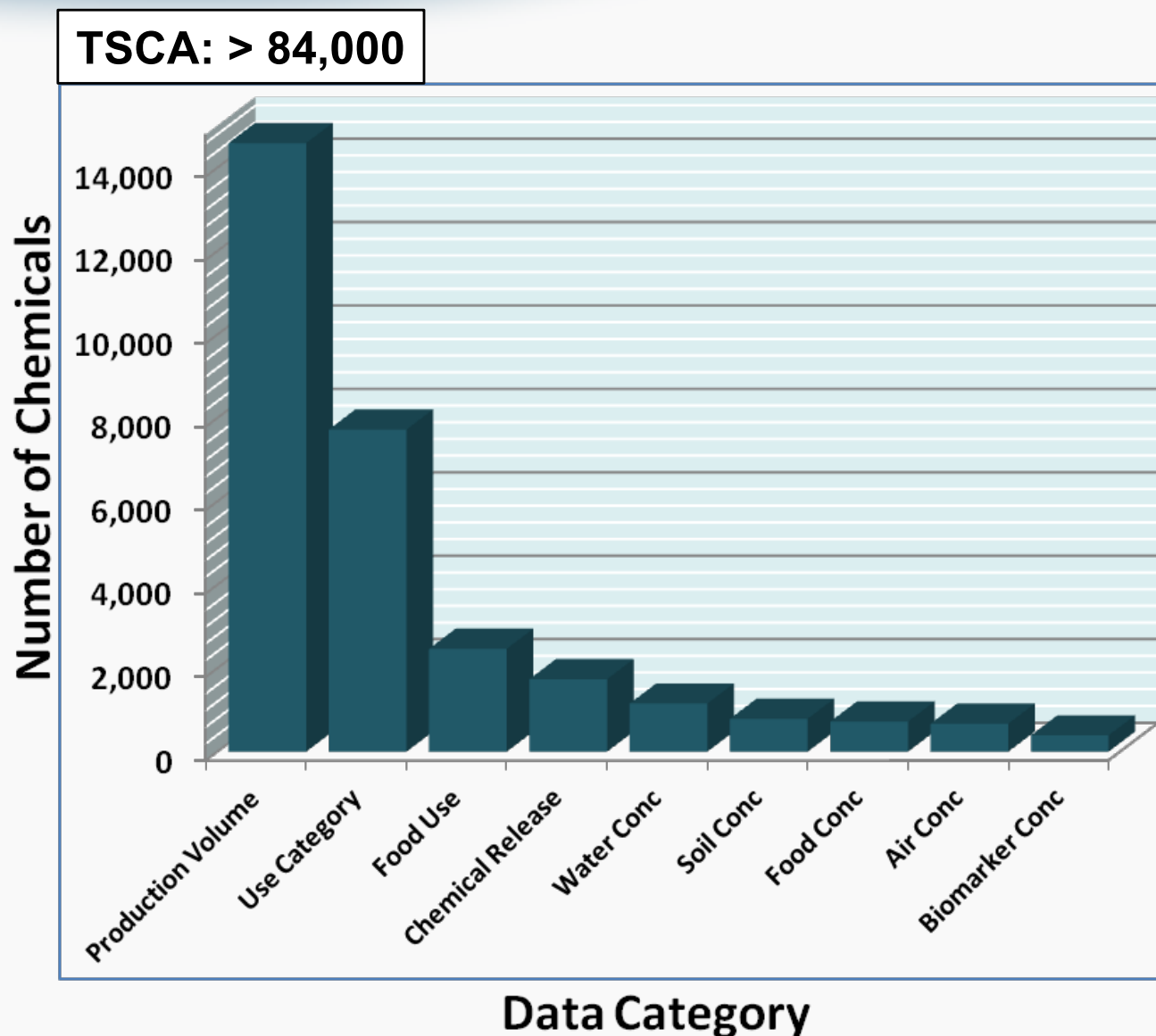
Who is NCCT?



- National Center for Computational Toxicology – part of EPA's Office of Research and Development
- Research driven by EPA's *Chemical Safety for Sustainability Research Program*
 - Develop new approaches to **evaluate the potential chemical toxicity**
 - Integrate advances in biology, biotechnology, chemistry, exposure science and computer science
- Goal - To identify environmental **chemical exposures** that may disrupt biological processes and cause adverse outcomes.



Exposure Data Has Not Kept Pace with Regulatory Needs



The CompTox Chemistry Dashboard: An Overview




- A **publicly accessible website** delivering access:
 - ~750,000 chemicals and related property data
 - Links to other agency websites and public data resources
 - “Literature” searches for chemicals using public resources
 - Integration to “biological assay data” for 1000s of chemicals
 - Information regarding consumer products containing chemicals
 - “Batch searching” for thousands of chemicals
- Day-to-day curation efforts for data quality


Comptox Chemistry Dashboard

<https://comptox.epa.gov>




 United States Environmental Protection Agency [Home](#) [Advanced Search](#)

Chemistry Dashboard Aa ▼ Aa Aa ▲



**~750,000 chemicals
>15 years of data**

Chemistry Dashboard



☐ Single component search ☐ Ignore isotopes



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

Need more? Use [advanced search](#).

741 Thousand Chemicals

Latest News

■ New CompTox Mobile app releases >700,000 chemicals on iPhone and iPad
January 20, 2017 at 8:40:18 AM

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Comptox Chemistry Dashboard

<https://comptox.epa.gov>



EPA United States Environmental Protection Agency Home Advanced Search

Chemistry Dashboard

~ 750,000 chemicals
>15 years of data

Chemistry Dashboard

Search a chemical by systematic name, synonym, CAS number, or InChIKey

☐ Single component search ☐ Ignore isotopes

See what people are saying, read the dashboard comments!

Need more? Use advanced search.

741 Thousand Chemicals

Latest News

■ New CompTox Mobile app releases >700,000 chemicals on iPhone and iPad
January 20, 2017 at 8:40:18 AM

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Comptox Chemistry Dashboard


<https://comptox.epa.gov>



EPA United States Environmental Protection Agency Home Advanced Search

Chemistry Dashboard

As A3 A3



**~750,000 chemicals
>15 years of data**

Chemistry Dashboard

- Atrazin
- atrazina
- Atrazine
- Atrazine de ethyl
- Atrazine Deisopropyl
- Atrazine de-isopropyl
- Atrazine mercapturate
- Atrazine hydrochloride
- Atrazine mixture with butylate
- Atrazine (6-Chloro-N-ethyl-N'-(1-methylethyl)1,3,5,-triazine-2,4-diamine)

Latest News

■ New CompTox Mobile app releases >700,000 chemicals on iPhone and iPad
January 20, 2017 at 8:40:18 AM

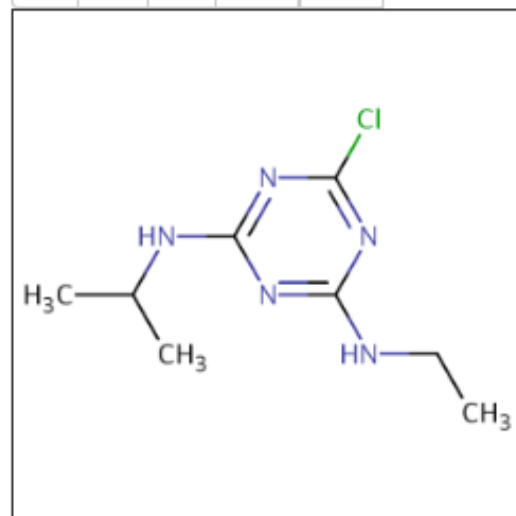
About Contact Privacy ACToR DSSTox Accessibility Help Downloads

Chemical Page

Atrazine

1912-24-9 | DTXSID9020112 ⓘ

ⓘ Searched by Approved Name: Found 1 result for 'atrazine'.



Wikipedia

Intrinsic Properties

Molecular Formula: C₈H₁₄ClN₅

Find All Chemicals



Average Mass: 215.69 g/mol



Monoisotopic Mass: 215.093773 g/mol



Structural Identifiers

Record Information

Chemical Properties

Synonyms

External Links

Product Composition

Bioassays

Exposure

Analytical

Literature

Comments

Physicochemical Properties

Summary

Download as:

TSV

Excel

SDF

LogP: Octanol-Wa...

Water Solubility

Density

Melting Point

Boiling Point

Surface Tension

Vapor Pressure

Soil Adsorp. Coeff.

LogKoa: Octanol-Air

Property	Average		Median		Range		Unit
	Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
LogP: Octanol...	2.61 (1)	2.66 (4)	2.61 to 2.61	2.66	2.61	2.50 to 2.82	-
Water Solubility	1.30e-04 (1)	1.46e-02 (4)	1.30e-04 to 1....	1.46e-02	1.30e-04	1.50e-04 to 5....	mol/L
Density	-	1.27 (1)	-	1.27	-	-	g/cm^3
Melting Point	174 (6)	151 (3)	173 to 177	151	173 to 177	114 to 187	°C
Boiling Point	-	312 (3)	-	312	-	284 to 339	°C
Surface Tension	-	53.8 (1)	-	53.8	-	-	dyn/cm
Vapor Pressure	7.21e-11 (1)	4.47e-06 (3)	7.21e-11 to 7....	4.47e-06	7.21e-11	2.03e-07 to 1....	mmHg
Soil Adsorp. C...	174 (1)	173 (2)	174 to 174	173	174	144 to 202	L/kg
LogKoa: Octa...	-	8.40 (1)	-	8.40	-	-	-
Henry's Law	-	4.20e-10 (1)	-	4.20e-10	-	-	atm-m3/mole
Atmos. Hydrox...	-	1.71e-11 (1)	-	1.71e-11	-	-	cm3/molecule*...

Chemical Properties

Synonyms

External Links

Product Composition

Bioassays

Exposure

Analytical


Literature

Comments

Names and Identifiers

Found 100 synonyms

Legend: **Valid Synonyms** *Good Synonyms* Other Synonyms

 Copy all Synonyms

Atrazine

1,3,5-Triazine-2,4-diamine, 6-chloro-N-ethyl-N'-(1-methylethyl)-

1912-24-9 **Active CAS-RN**

UNII-QJA9M5H4IM **FDA Registry Number**

1,3,5-Triazine-2,4-diamine, 6-chloro-N2-ethyl-N4-(1-methylethyl)-

1-Chloro-3-ethylamino-5-isopropylamino-2,4,6-triazine

2-Chloro-4-(ethylamino)-6-(2-propylamino)-s-triazine

2-Chloro-4-(ethylamino)-6-(isopropylamino)-s-triazine

2-Chloro-4-(ethylamino)-6-(isopropylamino)triazine

2-Chloro-4-ethylamineisopropylamine-s-triazine

2-Chloro-4-ethylamino-6-isopropylamino-1,3,5-triazine

2-Chloro-4-ethylamino-6-isopropylamino-s-triazine

2-Ethylamino-4-isopropylamino-6-chloro-s-triazine

6-Chloro-4-(ethylamino)-2-(isopropylamino)-s-triazine

6-Chloro-N-ethyl-N'-(1-methylethyl)-1,3,5-triazine-2,4-diamine

Chemical Properties

Synonyms

External Links

Product Composition

Bioassays

Exposure

Analytical


Literature

Comments

Active vs Deleted CASRN

Found 23 synonyms

Legend: **Valid Synonyms** *Good Synonyms* *Other Synonyms*

 Copy all Synonyms

7,7-Dimethyl-3-[(4-methylphenyl)methylidene]bicyclo[2.2.1]heptan-2-one

bicyclo[2.2.1]heptan-2-one, 7,7-dimethyl-3-[(4-methylphenyl)methylene]-

Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-3-[(4-methylphenyl)methylene]-

36861-47-9 **Active CAS-RN**

UNII-8I3XWY40L9 **FDA Registry Number**

EINECS 253-242-6

Eusolex 6300

Uvinul MBC 95

Parsol 5000

Neo Heliopan MBC

3-(p-Methylbenzylidene)camphor

3-(p-Methylbenzylidene)-DL-camphor

3-(4-Methylbenzylidene)camphor

3-(4-Methylbenzylidene)-DL-camphor

3-(4'-Methylbenzylidene)camphor

3-(p-Methylbenzylidene)bornan-2-one

1,7,7-Trimethyl-3-(4-methylbenzylidene)bicyclo(2.2.1)heptan-2-one

4-Methylbenzylidenecamphor

p-Methylbenzylidenecamphor

38102-62-4 **Deleted CAS-RN**

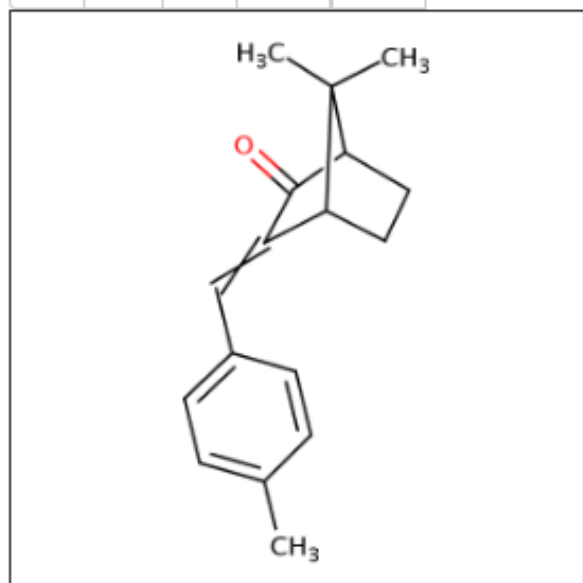
84055-65-2 **Deleted CAS-RN**

Collisions in CAS Numbers

Enzacamene


36861-47-9 | DTXSID8047896 

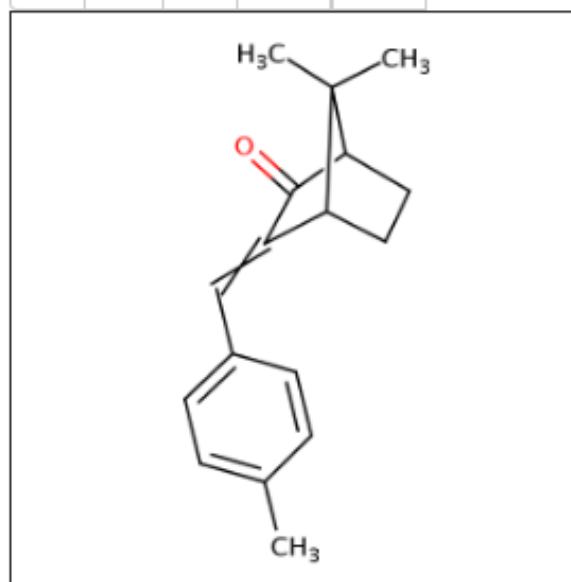
 Searched by CAS-RN: Found 1 result for '36861-47-9'.



Enzacamene

36861-47-9 | DTXSID8047896 

 Searched by Deleted CAS-RN: Found 1 result for '38102-62-4'.

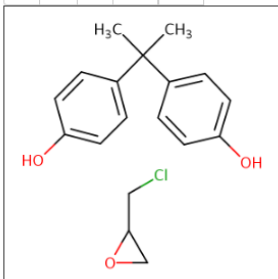
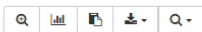


How Bad Can It Get??

Bisphenol A/ Epichlorohydrin resin

25068-38-6 | DTXSID0050479 ⓘ

ⓘ Searched by CAS-RN: Found 1 result for '25068-38-6'.



Intrinsic Properties

Molecular Formula: C₁₈H₂₁ClO₃

Average Mass: 320.81 g/mol

Monoisotopic Mass: 320.117922 g/mol

Structural Identifiers

Record Information

Found 664 synonyms

Legend: **Valid Synonyms** *Good Synonyms* *Other Synonyms*  Copy all Synonyms

1096473-97-0 Deleted CAS-RN
110158-22-0 Deleted CAS-RN
11097-80-6 Deleted CAS-RN
11098-13-8 Deleted CAS-RN
11098-40-1 Deleted CAS-RN
11100-23-5 Deleted CAS-RN
11108-41-1 Deleted CAS-RN
11120-31-3 Deleted CAS-RN
11121-19-0 Deleted CAS-RN
11126-36-6 Deleted CAS-RN
1114797-08-8 Deleted CAS-RN
111517-59-0 Deleted CAS-RN
114013-37-5 Deleted CAS-RN
115902-32-4 Deleted CAS-RN
117216-90-7 Deleted CAS-RN
117786-92-2 Deleted CAS-RN
118340-04-8 Deleted CAS-RN
1189565-70-5 Deleted CAS-RN
1190235-62-1 Deleted CAS-RN
1190729-68-0 Deleted CAS-RN
1192045-32-1 Deleted CAS-RN

How Bad Can It Get?

This one is **316** Deleted CASRN



CAS Registry Number: 25068-38-6

(C₁₅H₁₆O₂ · C₃H₅ClO)_x

Phenol, 4,4'-(1-methylethylidene)bis-, polymer with 2-(chloromethyl)oxirane

Polymer














Polymer Class Terms: Epoxy resin

Alternate CAS Registry Numbers: 26402-79-9














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Links to Other Resources











General

 EPA Substance Re...
 NIST Chemistry W...
 Household Product...
 PubChem
 Chemspider
 CPCat
 DrugBank
 HMDB
 Wikipedia
 MSDS Lookup
 ChEMBL
 Chemical Vendors
 Consumer Product...






Toxicology

 ACToR
 DrugPortal
 CCRIS
 ChemView
 CTD
 e
 E
 G
 HSDB
 ToxCast Dashboar...
 LactMed
 ACToR PDF Report
 International Toxicit...

Publications

 Toxline
 Environmental Heal...
 NIEHS
 National Toxicology...
 Google Books
 Federal Register
 Regulations.gov
 Springer Materials
 BioCaddie DataMed
 RSC Publications

Analytical

 National Environme...
 MONA: MassBank ...
 Tox21 Analytical Data
 RSC Analytical Abs...
 FOR-IDENT

The Office of the Federal Register (OFR) of the National Archives and Records Administration (NARA), and the U.S. Government Printing Office (GPO) jointly administer the FederalRegister.gov website.

Chemical Properties

Synonyms

External Links

Product Composition

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Literature

Comments

Example External Links...

**ChemHAT.org**
Chemical Hazard and Alternatives Toolbox

English | Español

ABOUT CHEMHAT SAFER CHEMICALS FOR WORKERS BREAST CANCER SAFER FAMILIES

Atrazine
CAS: 1912-24-9

Stronger effect / evidence     Weaker effect / evidence

How can this chemical affect my health?

■ Acute (Short Term) Effects [Data sources](#) 

**Toxic to Humans & Animals** – Can be fatal on contact, ingestion or inhalation for humans and other mammals.

**Irritates the Eyes** – Can cause irritation or serious damage to the eye.

■ Chronic (Long Term) Effects [Data sources](#) 

**Birth Defects** – Can cause harm to the developing child including birth defects, low birth weight and biological or behavioral problems that appear as the child grows.

**Reproductive Harm** – Can disrupt the male or female reproductive systems, changing sexual development, behavior or functions, decreasing fertility, or resulting in loss of the fetus during pregnancy.

**Endocrine Disruption** – Can interfere with hormone communication between cells which controls metabolism, development, growth, reproduction and behavior (the endocrine system).

**Sensitizes the Skin** – Can lead to allergic reactions on the skin.

**Other Health Effects** – Can cause serious damage on contact or ingestion.

**Cancer** – Can cause or increase the risk of cancer.

**Breast Cancer** – Known to increase mammary gland tumors in animals.

Example External Links...



All

HOME ABOUT CPID PRODUCT RECALLS CONTACT US SEARCH ALL

cpid

Consumer Product Information Database
Health effects of consumer products

What's in it? ▶ Search Entire CPID Database

Enter Products, Manufacturers, Chemicals, Product Categories and Product Types

GO

▶ Advanced Search

You may also search by:

▶ Brands ▶ Product Type ▶ Ingredients ▶ Manufacturers ▶ Health Effects - (M)SDS ▶ First Aid

Atrazine

Primary Chemical Name :	Atrazine
CAS Registry Number:	001912-24-9
EC Number:	217-617-8
Synonyms:	2-Chloro-4-(2-propylamino)-6-ethylamino-s-triazine; 2-Chloro-4-ethylamino-6-isopropylamino-s-triazine; 2-Chloro-4-ethylamino-6-isopropylamino-1,3,5-triazine; 2-Chloro-4-ethylamineisopropylamine-s-triazine; 2-Ethylamino-4-isopropylamino-6-chloro-s-triazine; s-Triazine, 2-chloro-4-ethylamino-6-isopropylamino-; 1-Chloro-3-ethylamino-5-isopropylamino-2,4,6-triazine
SVHC?:	No

Chemical Structure

Health Studies

Toxicity Studies

Biomedical Reference

ECHA - Chem

GHS Classification

Properties and Health Effects

Product Composition Details



Download as:

TSV

Excel

Product Composition

Product	Percent Composition ↓	Manufacturer
PS-380 ATRAZINE, 99.5% PURE	99.5%	CHEM SERVICE INC
ATRAZINE 80W	76.0%	ACETO AGRICULTURAL CHEMICALS CORP
ATRATOL 80W	71.3%	CIBA-GEIGY CORPORATION
ATRATOL 8P	8%	CIBA-GEIGY CORP
LPC-507M LAB PERFORMANCE CHECK MIXTURE IN T-B...	<1%	CHEM SERVICE INC
F2208S 2-CHLORO-4-ETHYLAMINO-S-TRIAZINE 100 UG...	<1%	CHEM SERVICE INC
ST84798, PROTURF ST AUGUSTINE WEED CONTROL	0.99%	O M SCOTT & SONS CO
SCOTTS BONUS, 26-3-3	0.94%	O. M. SCOTT & SONS CO.
SCOTTS LAWN PRO SUPER BONUS S, 21-3-3	.57%	O. M. SCOTT & SONS CO.
10-3-3 FERTILIZER + ATRAZINE	0.42%	ESTECH BRANDED FERTILIZERS, INC

Chemical Properties

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Comments

In vitro Bioassay Data

- *In vitro* **bioassays** are used to determine the biological activity of a substance – **ToxCast and Tox21 projects**
- A decade of measurements, and millions of dollars of data integrated into the dashboard

NVS_GPCR_hAdoRA1

Assay Name: NVS_GPCR_hAdoRA1

Gene Symbol: ADORA1

Organism: human

Tissue: brain

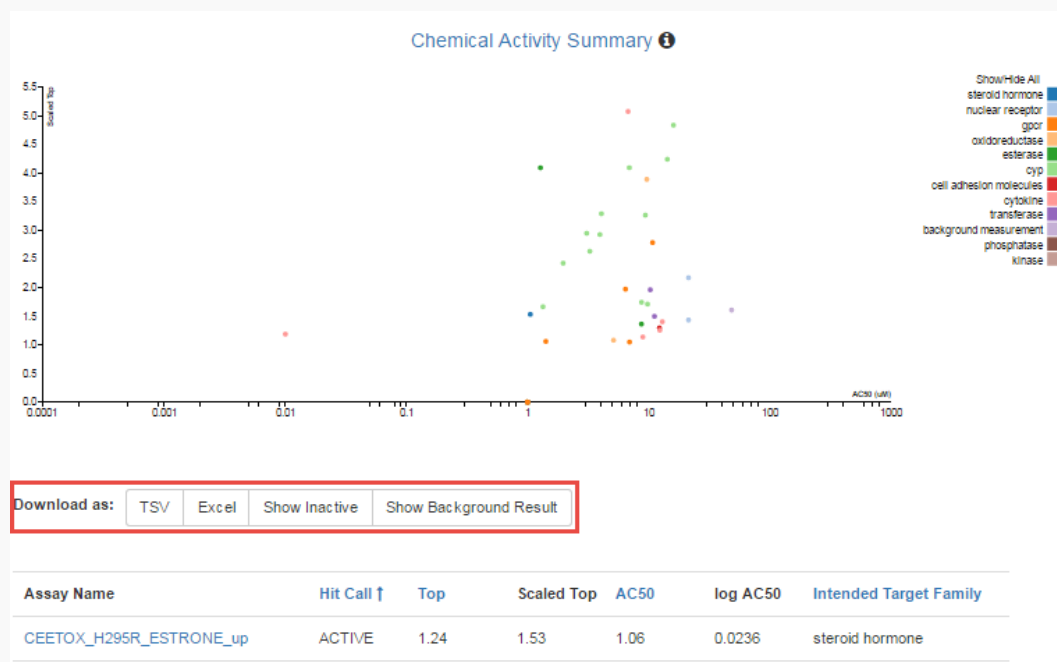
Assay Format Type: biochemical

Biological Process Target: receptor binding

Detection Technology: Radiometry

Analysis Direction: positive

Intended Target Family: gpcr



Chemical Properties

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Integrated Literature Searching



PubChem



BioAssay ?



Compound ?



Substance ?

Google
Scholar

atrazine

PubMed

PubMed comprises more than 26 million citations for biomedical literature from MEDLINE, life science journals, and online books. Citations may include links to full-text content from PubMed Central and publisher web sites.

Chemical Properties

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Integrated Literature Searching



PubChem Artic...

Google Scholar

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PubChem Patents

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PUBCHEM > COMPOUND > ATRAZINE > LITERATURE > DEPOSITOR PROVIDED PUBMED CITATIONS >

Depositor Provided PubMed Citations

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1 to 10 of 876

1 2 3 ... 88

Date

PMID	Date	Title	Journal
26923738	2016-06-01	Atrazine blocks ovulation via suppression of Lhr and Cyp19a1 mRNA and estradiol secretion in immature gonadotropin-treated rats.	Reproductive toxicology (Elmsford, N.Y.)
27114639	2016-03-01	Atrazine exposure causes mitochondrial toxicity in liver and muscle cell lines.	Indian journal of pharmacology
26647222	2016-01-05	Endocrine-Disrupting Effects of Pesticides through Interference with Human Glucocorticoid Receptor.	Environmental science & technology
26464060	2016-01-01	Effects of Neonicotinoids on Promoter-Specific Expression and Activity of Aromatase (CYP19) in Human Adrenocortical Carcinoma (H295R) and Primary Umbilical Vein Endothelial (HUVEC) Cells.	Toxicological sciences : an official journal of the Society of Toxicology
26377646	2015-09-16	Atrazine-Mediated Disruption of Steroidogenesis in BLTK1 Murine Leydig Cells.	Toxicological sciences : an official journal of the Society of Toxicology

Chemical Properties

Synonyms

External Links

Product Composition

Bioassays

Exposure

Analytical

Literature

Comments

Integrated Literature Searching



Google Scholar

Abstract Sifter

PubChem Articles

PubChem Patents

IRIS

Select Term: Hazard AND RfD OR reference dose AND -

Edit the Query Before Querying (66 Characters)

"RfD OR reference dose" AND "Hazard" AND "1912-24-9" OR "Atrazine"

Submit

Google

"RfD OR reference dose" AND "Hazard" AND "1912-24-9" OR "Atrazine"

Scholar

About 579 results (0.06 sec)

Articles

Case law

My library

Any time

Since 2017

Since 2016

Since 2013

Custom range...

Sort by relevance

Sort by date

☒ include patents

☒ include citations

☒ Create alert

Pesticide management in food and water safety: international contributions and national approaches

G Ekström, M Åkerblom - Reviews of environmental contamination and ..., 1990 - Springer

... Acute **hazard** unlikely **Atrazine** Benomyl Butachlor Butylate Carbendazim Carboxin Chlormethoxyfen Chloridazon Chlorothalonil Diuron ... EPA **reference dose** data reprinted with permission from the US EPA ... a Classified by WHO as unlikely to produce acute **hazard** in nor- ...

Cited by 31 Related articles All 6 versions Web of Science: 18 Cite Save More

Immunotoxic effects of short-term atrazine exposure in young male C57BL/6 mice

NM Filipov, LM Pinchuk, BL Boyd... - Toxicological ..., 2005 - Soc Toxicology

... Moreover, documented exposures of over 200,000 people to **atrazine** levels above the acute **Reference Dose** (RfD) have been reported ... **Atrazine** disrupts the hypothalamic control of pituitary-ovarian function. ... Third report on the **hazard** identification assessment review committee ...

Cited by 71 Related articles All 14 versions Web of Science: 47 Cite Save More

Health risks of heavy metals to the general public in Tianjin, China via consumption of vegetables and fish

X Wang, T Sato, B Xing, S Tao - Science of the Total Environment, 2005 - Elsevier

... exposures. These are typically based on the target **hazard** quotient (THQ), which is a ratio of determined dose of a pollutant to the dose level (a **Reference Dose** or RfD). If the ratio is less than 1, there will not be any obvious risk. ...

Cited by 517 Related articles All 7 versions Web of Science: 269 Cite Save More

Non-occupational exposures to pesticides for residents of two US cities

RW Whitmore, FW Immerman, DE Camann... - Archives of ..., 1994 - Springer

https://www.google.com/search?tbm=isch&q="RfD+OR+reference+dose"+AND+... alonil (Bravo ©) 0.5-2.5 X Folpet 0.5-37.0 X

Chemical Properties

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Bioassays

Exposure

Analytical

Literature

Comments

Integrated Literature Searching



Google Scholar

Abstract Sifter

PubChem Articles

PubChem Patents

IRIS

Select Term:

Select a Query Term ▼

Retrieve Articles

0 Articles

Edit the Query Before Retrieving Articles

"1912-24-9" OR "Atrazine" OR "Atrazine"

Add additional query terms to filter abstracts:

Search and Count

Select Term:

Select a Query Term ▼

Select a Query Term

- Hazard
- Fate and Transport
- Metabolism/PK/PD
- Chemical Properties
- Exposure
- Mixtures
- Male Reproduction
- Androgen Disruption
- Female Reproduction
- GeneTox
- Embryo and embryonic development
- Child (infant through adolescent)
- Dust and Exposure

Chemical Properties

Synonyms

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Product Composition

Bioassays

Exposure

Analytical

Literature

Comments

Integrated Literature Searching

Select Term:

Hazard

Retrieve Articles

28 Articles (out of 28)

Edit the Query Before Retrieving Articles

("1912-24-9" OR "Atrazine" OR "Atrazine") AND (NOAEL or NOEL OR LOEL or Rfd OR "reference dose" OR "reference concentration" OR "adverse effect level" [tiab] OR "cancer slope factor"[tiab])

Add additional query terms to filter abstracts:

estrogen

endocrine

Search and Count

est...	end...	Ter...	Total	PMID	Pub..	Title
3	1	0	4	10613397	1999	Estrous cycle patterns of Sprague-Dawley rats during acute and chronic atrazine administration.
2	1	0	3	15655806	2005	A risk assessment of atrazine use in California: human health and ecological aspects.
1	1	0	2	15590006	2004	Impact of endocrine toxicants on survival, development, and reproduction of the estuarine copepod Eurytemora affinis...
0	1	0	1	8829248	1996	Effect of atrazine on ovarian function in the rat.
0	0	0	0	28089211	2017	Toxicity effects of an environmental realistic herbicide mixture on the seagrass Zostera noltei.

Record:   1 of 28  

Title: Effect of atrazine on ovarian function in the rat.

Abstract: The effect of the chlorotriazine herbicide, atrazine, on ovarian function was studied in Long-Evans hooded (LE-hooded) and Sprague-Dawley (SD) rats. Atrazine was administered by gavage for 21 d to females displaying regular 4-d estrous cycles. In both strains, 75 mg/kg/d disrupted the 4-d ovarian cycle; however, no distinct alteration (i.e., irregular cycles but not persistent estrus or diestrus) was apparent at this dose. At 150 mg/kg/d, atrazine induced repetitive pseudopregnancies in females of both strains. The highest dose tested (300 mg/kg/d) also induced repetitive pseudopregnancies in the SD females, while the ovaries of the LE-hooded female appeared regressed and the smear cytology was indicative of the anestrus condition. Although a NOAEL was not established, the doses employed in this experiment were in excess of those used in chronic feeding studies in which an early onset of mammary gland tumors was noted. These data demonstrate that atrazine can disrupt ovarian function and bring about major changes in the **endocrine** profile of the female.

Chemical Properties

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Exposure

Analytical

Literature

Comments

Integrated Literature Searching

Select Term:

Hazard

Retrieve Articles

28 Articles (0)

Add additional query terms to filter

estrogen

Edit the Query Before Retrieving Articles

("1912-24-9" OR "Atrazine" OR "Atrazine") AND (NOAEL or NOEL OR LOEL or Rfd OR "reference dose" OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])

est...	end...	Ter...	Total	PMID	Pub..	Title
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Record:



1 of 28



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28 Articles (out of 28)

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("1912-24-9" OR "Atrazine" OR "Atrazine") AND (NOAEL or NOEL OR LOEL or Rfd OR "reference dose" OR "reference concentration" OR "adverse effect level" [tiab] OR "cancer slope factor"[tiab])

Add additional query terms to filter abstracts:

estrogen

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est...	end...	Ter...	Total	PMID	Pub..	Title
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Atrazine was
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e highest dose tested
y was indicative of the
an early onset of
female.

Chemical Properties

Synonyms

External Links

Product Composition

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Comments

Crowdsourced Data Curation

- Maintaining high-quality data is a challenge
- Every user can contribute to improving the data!

[Submit Comment](#)

New Comment ×


Comment

The chemical name associated with this structure is not correct. This is the citrate salt.

Email address

Enter your email address

☐ I'm not a robot


reCAPTCHA
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Submit

Chemical Properties

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Literature

Comments

“Not just structures”

Poly (acrylamide-co-acrylic acid), partial sodium salt

62649-23-4 | DTXSID1049722 ⓘ

ⓘ Searched by Approved Name: Found 1 result for 'Poly (acrylamide-co-acrylic acid), partial sodium salt'.

Record Information

Citation

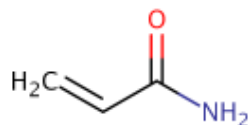
U.S. Environmental Protection Agency. Chemistry Dashboard. <https://comptox.epa.gov/dashboard/DTXSID1049722> (accessed February 12, 2017), Poly (acrylamide-co-acrylic acid), partial sodium salt

Data Quality **80%**

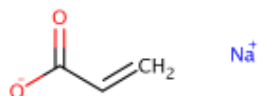
Manually curated and no conflicts in multiple public sources

Related Chemicals

Found 2 chemicals



Acrylamide
79-06-1



2-Propenoic acid, sodium salt
7446-81-3

Batch Searching for Data for Thousands of Chemicals

- What are these chemicals?

Chemicals Used in the Hydraulic Fracturing Process in Pennsylvania Prepared by the Department of Environmental Protection Bureau of Oil and Gas Management

Updated June 10, 2010

Chemical	Product Name
2,2-Dibromo-3-Nitrilopropionamide	Bio Clear 1000/Bio Clear 2000/ Bio-Clear 200/BioRid20L/ EC6116A
2-methyl-4-isothiazolin-3-one	X-Cide 207
5-chloro-2-methyl-4-isothiazolin-3-one	X-Cide 207
Acetic Acid	Fe-1A Acidizing Composition/ Packer Inhibitor
Acetic Anhydride	Fe-1A Acidizing Composition
Acetylene	GT&S Inc./ Airco
Alcohol Ethoxylated	C12-16 NE-200
Alkyl benzene sulfonic acid	Tetrolite AW0007/ FR-46
Ammonia (aqueous)	FAW-5
Ammonium Bifluoride	ABF 37%
Ammonium Persulfate	AP Break
Ammonium Bisulfite	Techni-Hib 604/ Fe OXCLEAR/ Packer Inhibitor
Ammonium chloride	Salt Inhibitor
Ammonium Salt (alkylpolyether	

Batch Searching for Data for Thousands of Chemicals

Select Input Type(s)

- ☒ Chemical Name
- ☐ CAS-RN
- ☐ InChIKey
- ☐ DSSTox Substance ID
- ☐ Exact Molecular Formula ⓘ

Enter Identifiers to Search

Sodium l-glutamate
4-Hydroxy-3-nitrophenylarsonic acid
4-Nitro-1,2-phenylenediamine
Methoxypromazine
1-Phenyl-3-methyl-5-pyrazolone
1-Phenyl-2-thiourea
Phenylbutazone
1,4-Benzenediamine
Prednisolone
Probenecid

Display All Chemicals

Download Chemical Data

Select Output Format


Excel ▼

Customize Results

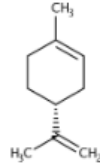

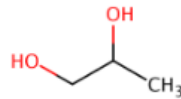
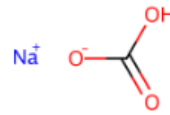
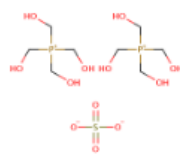
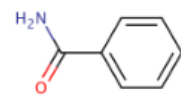


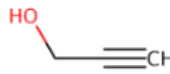
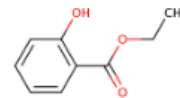


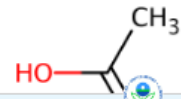
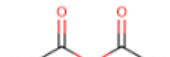

☐ Select All

Chemical Identifiers	Structures	Intrinsic Properties
<input checked="" type="checkbox"/> Chemical Name	<input type="checkbox"/> Mol File	<input type="checkbox"/> Molecular Formula
<input checked="" type="checkbox"/> DTXSID	<input type="checkbox"/> SMILES	<input type="checkbox"/> Average Mass
<input type="checkbox"/> CAS-RN	<input type="checkbox"/> InChI String	<input type="checkbox"/> Monoisotopic Mass
<input type="checkbox"/> InChIKey		<input type="checkbox"/> OPERA and TEST Model Predictions
<input type="checkbox"/> IUPAC Name		

Access to associated data for review, modeling & download



 United States Environmental Protection Agency [Home](#) [Advanced Search](#)

Chemistry Dashboard



 D-Limonene 5989-27-5	 Potassium chloride 7447-40-7	 1,2-Propylene glycol 57-55-6	 Sodium bicarbonate 144-55-8	 Tetrakis(hydroxymethyl)phospho... 55566-30-8
 Benzamide 55-21-0	 Methanol 67-56-1	 1-Butanol 71-36-3	 Propargyl alc ohol 107-19-7	 Ethyl salicylate 118-61-6
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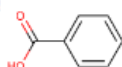

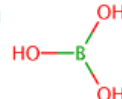

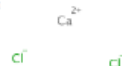

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Chemistry Dashboard

[View Selected](#) [Hide Isotopes](#) [Hide Multicomponent Chemicals](#)   [Aa ▼](#) [Aa](#) [Aa ▲](#)

 Searched by List: Found 64 results.

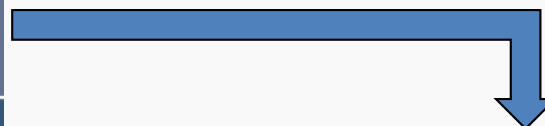
Download as: [TSV ▼](#) [Excel ▼](#) [SDF ▼](#)

ID ↑↓	Structure	Preferred Name ↑↓	CAS-RN ↑↓	QC Level ↑↓	CPCat C...	Number...	PubChe...	Monoisotopic M...	
DTXSID0020078		Ammonium chloride	12125-02-9	DSSTox High	561	28	82	53.003227	
DTXSID6020143 ToxCast™		Benzoic acid	65-85-0	DSSTox High	87	70	441	122.036779	
DTXSID1020194 ToxCast™		Boric acid	10043-35-3	DSSTox High	792	51	142	62.017524	
DTXSID5020235 ToxCast™		Calcium chloride	10043-52-4	DSSTox High	294	33	81	109.900296	

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Real World Applications

- From chemical names to chemical data



Anthracene		120-12-7
Aromatic oil		
9,10-Anthracenedione, 2-ethyl	2-Ethylantracene-9,10-dione	84-51-5
Azobenzene		103-33-3
Benz(e)acenaphthylene	Acephenanthrylene	201-06-9
Benzaldehyde, 3-hydroxyl-4-methoxy	3-Hydroxy-4-methoxy-benzaldehyde	621-59-0
Benz(a)anthracene		56-55-3
Benzene		71-43-2
Benzene, 1,3-bis(1-methylethenyl)-	1,3-bis(1-methylethenyl)benzene; 1,3-Diisopropenylbenzene	3748-13-8
Benzene, 1,4-bis(1-methylethenyl)-	1,4-Bis(1-methylethenyl)benzene	1605-18-1
1,4-Benzenediamine, N,N'-diphenyl-	N,N'-Diphenyl-p-phenylenediamine	74-31-7

Download as: [TSV](#) [Excel](#) [PDF](#)

ID	Preferred Name	CAS RN	QC Level	Number of Sources	PubChem Data Source Count
Monocyclic Aromatic					
1	Azobenzene	103-33-3			
2	N,N'-Diphenyl-p-phenylenediamine	74-31-7			
3	1,3-Diisopropenylbenzene	3748-13-8			
4	Benzene-D6	1076-43-3			
5	1,4-Bis(1-methylethenyl)benzene	1605-18-1			
6	Benzene	71-43-2			
7	2-Ethylantracene-9,10-dione	84-51-5			
8	3-Hydroxy-4-methoxybenzaldehyde	621-59-0			
9	2,6-Anthracenedithione acid, 9,10-dihydro-9,10-dioxo-	84-50-4			
10	Acephenanthrylene	201-06-9			



Data Available for Download

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



Downloads

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

Posted: 11/14/2016

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

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

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

Posted: 11/14/2016

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

	A	B	
1	casrn	dsstox_substance_id	preferred_name
2	26148-68-5	DTXSID7020001	A-alpha-C
3	107-29-9	DTXSID2020004	Acetaldehyde oxime
4	60-35-5	DTXSID7020005	Acetamide
5	103-90-2	DTXSID2020006	Acetaminophen
6	968-81-0	DTXSID7020007	Acetohexamide

~720,000 structures on iOS

CompTox Mobile

View in iTunes

+ This app is designed for
both iPhone and iPad

Free

Category: Productivity
Released: Jan 16, 2017
Version: 1.0
Size: 267 MB
Language: English
Seller: Kirill Blinov
© 2017 Molecule Apps,
2017 EPA
Rated 4+

Compatibility: Requires iOS 6.0
or later. Compatible with
iPhone, iPad, and iPod touch.

Customer Ratings

We have not received enough
ratings to display an average for
the current version of this
application.

More by Kirill Blinov



NMR

View in Mac App Store

Description

Find chemical structure instantly by exact mass (m/z), ^{13}C NMR chemical shifts, structure name or CAS Registry Number in a database of about 720,000 EPA CompTox structures.

[Kirill Blinov Web Site](#) > [CompTox Mobile Support](#) >

...More

Screenshots

iPhone | iPad

Future Work

- Continue expansion and curation of data and types.
- Provide “**programmatic access**” to all data – connect to other Agency resources and allow other scientists to integrate their scientific applications.
- Continue to assemble and enhance chemical lists and data for specific projects. Make available to Agency researchers and for public use.
- Integration of Global Health and Safety Data

Conclusion



- The CompTox Chemistry Dashboard provides access to data for ~750,000 chemicals
- An **Integration Hub** to data – toxicity, environmental, property, bioassay, and expanding
- Data downloads allows for reuse in other systems and integration of resources to support research

Antony Williams

US EPA Office of Research and Development

National Center for Computational Toxicology (NCCT)

Williams.Antony@epa.gov

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