

PubChem: A resource for chemical health and safety

Evan Bolton, Ph.D.


Disclaimer

- NLM does not endorse or recommend any commercial products, processes, or services. The views and opinions expressed do not necessarily state or reflect those of the U.S. Government, and they may not be used for advertising or product endorsement purposes.
- It is not the intention of NLM to provide specific medical advice, but rather to provide information to better understand health and disease. Specific medical advice will not be provided, and NLM urges you to consult with a qualified health professional for diagnosis and for answers to your personal medical questions.

PubChem is a data repository

- World's largest collection of freely accessible chemical information.
- Helps researchers make sense of the biological roles and health effects of chemicals on human health and the environment.


Chemical substances and bioactivities .. with select annotation

 National Library of Medicine
National Center for Biotechnology Information

PubChem [About](#) [Docs](#) [Submit](#) [Contact](#)

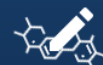
Explore Chemistry


Quickly find chemical information from authoritative sources





Try [covid-19](#) [aspirin](#) [EGFR](#) [C9H8O4](#) [57-27-2](#) [C1=CC=C\(C=C1\)C=O](#) [InChI=1S/C3H6O/c1-3\(2\)4/h1-2H3](#)

☐ Use Entrez ☐ Compounds ☒ Substances ☐ BioAssays

 Draw Structure

 Upload ID List

 Browse Data

 Periodic Table

116M Compounds 308M Substances 292M Bioactivities 36M Literature 932 Data Sources

[See More Statistics >](#) [Explore Data Sources >](#)

<https://pubchem.ncbi.nlm.nih.gov/>

Many page types

- Compound
- Gene
- Protein
- BioAssay
- Substance
- Patent
- Pathway,
Taxonomy,
Cell-line,
and more

PubChem Dopamine (Compound)

<https://pubchem.ncbi.nlm.nih.gov/compound/Dopamine>

PubChem ATP13A2 - ATPase cation transporting 13A2 (human) (Gene)

<https://pubchem.ncbi.nlm.nih.gov/gene/23400>

PubChem PDZ domain-containing protein 11 (Protein)

<https://pubchem.ncbi.nlm.nih.gov/protein/Q5EBL8>

PubChem siRNA Circadian Assay (BioAssay)

<https://pubchem.ncbi.nlm.nih.gov/bioassay/1904>

PubChem GNF169433 (Substance)

<https://pubchem.ncbi.nlm.nih.gov/substance/85115249>

PubChem COMPOSITIONS AND METHODS FOR TREATMENT OF NEU... (Patent)

<https://pubchem.ncbi.nlm.nih.gov/patent/US2017035860>

PubChem Ion channel transport (Pathway)

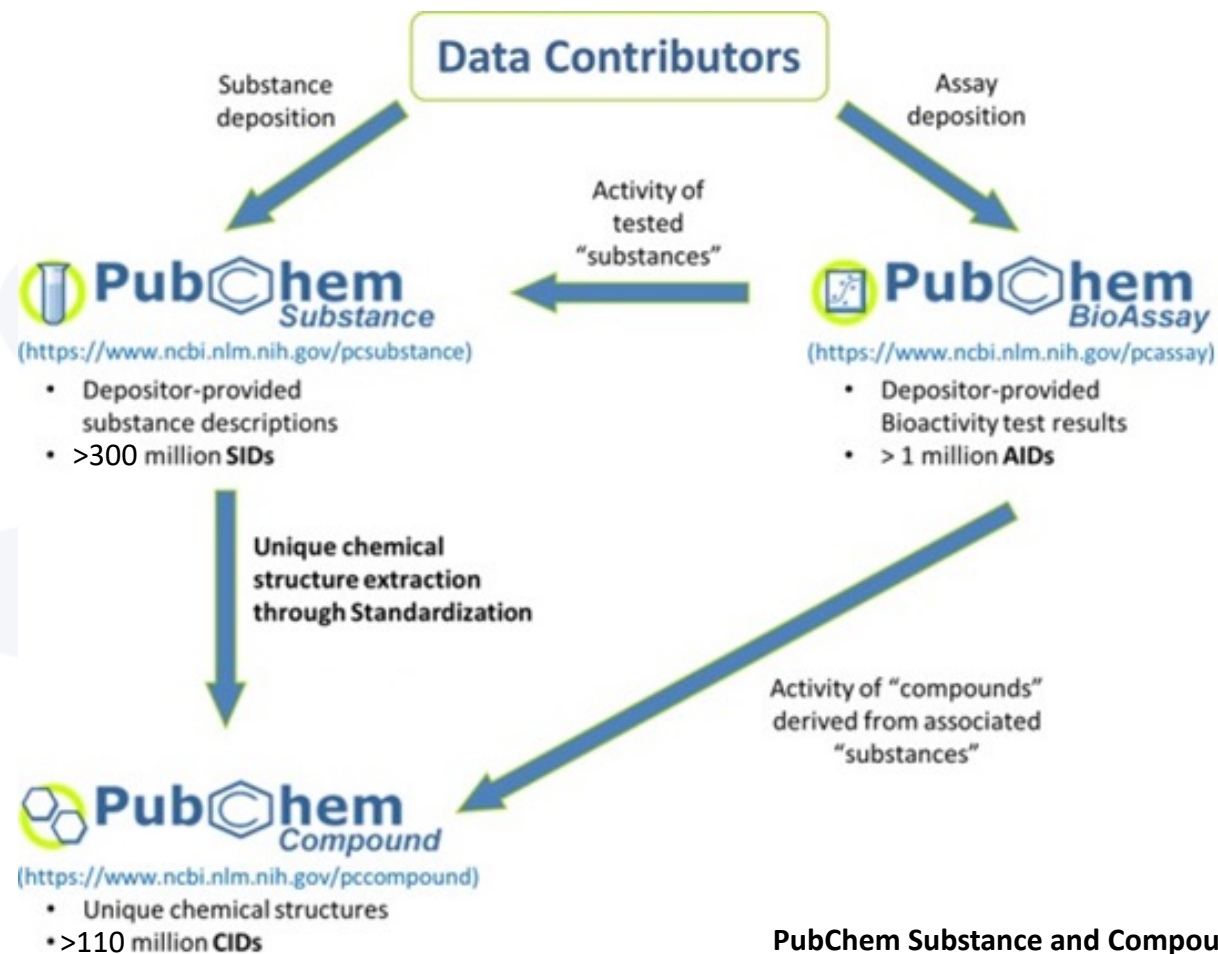
<https://pubchem.ncbi.nlm.nih.gov/pathway/Reactome:R-HSA-983712>

A lot of data ..
enabling
many
use cases

PubChem Data Counts

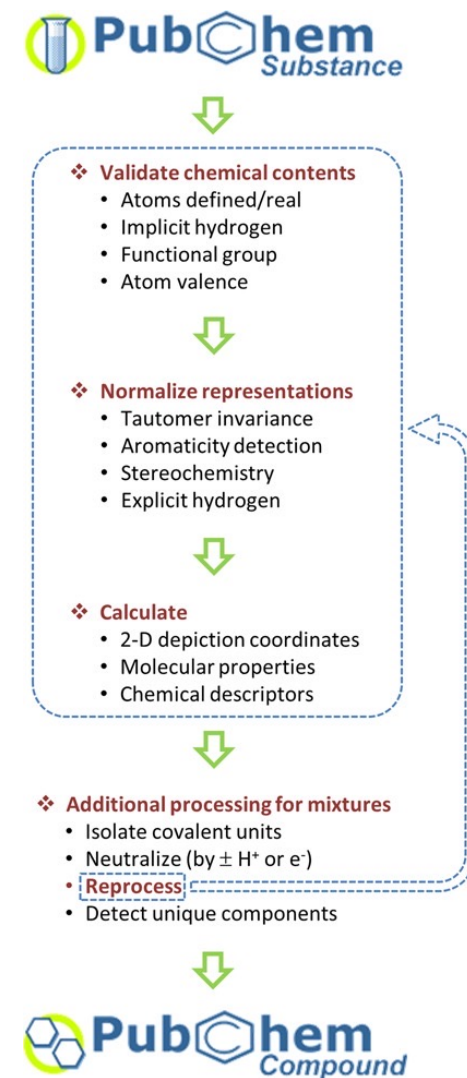
Collection	Live Count	Description
Periodic Table of Elements	118	Interactive periodic table with up-to-date element property
Compounds	115,668,812	Unique chemical structures extracted from contributed Pub
Substances	307,633,237	Information about chemical entities provided by PubChem
BioAssays	1,626,630	Biological experiments provided by PubChem contributors
Bioactivities	292,123,746	Biological activity data points reported in PubChem BioAss
Genes	112,728	Gene targets tested in PubChem BioAssays and those invol
Proteins	186,035	Protein targets tested in PubChem BioAssays and those inv
Taxonomy	113,693	Organisms of targets tested in PubChem BioAssays and th
Pathways	240,671	Interactions between chemicals, genes, and proteins
Cell Lines	1,986	Information about cell lines
Literature	38,884,316	Scientific publications with links in PubChem
Patents	42,020,426	Patents with links in PubChem
Data Classifications	71	Browse the distribution of PubChem data among nodes in
Data Sources	932	Organizations contributing data to PubChem

Two primary archival databases



PubChem Substance and Compound databases
Nucleic Acids Res. 2016 Jan 4;44(D1):D1202-13.
[DOI: 10.1093/nar/gkv951](https://doi.org/10.1093/nar/gkv951)
[PMID: 26400175](https://pubmed.ncbi.nlm.nih.gov/26400175/)
[PMCID: PMC4702940](https://pubmed.ncbi.nlm.nih.gov/26400175/pmc/articles/PMC4702940/)

Compound is derived from Substance



Compound Summary

- Top-level summary
- Nested navigation menu
- >500 different data fields
 - Experimental properties, Spectra, Literature, Toxicity, Bioactivities, Chemical vendors, Pharmacology, Patents, Pathways, Health & Safety, Classifications, ...
- Clear provenance
- Annotation from authoritative and curated sources

Toluene

” Cite

Download

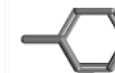
See also: [Benzene, toluene, ethylbenzene and xylene](#) (component of); [Benzene, toluene and xylene](#) (component of); [Laboratory-grade xylene](#) (impurity of).

PubChem CID 1140

Structure



2D



3D



Crystal

Chemical Safety



Flammable



Irritant



Health Hazard

[Laboratory Chemical Safety Summary \(LCSS\) Datasheet](#)

Molecular Formula

C_7H_8
 $C_6H_5CH_3$

Synonyms

toluene
methylbenzene
toluol
108-88-3
Phenylmethane

[View More...](#)

Molecular Weight

92.14 g/mol
Computed by PubChem 2.2 (PubChem release 2021.10.14)

Dates

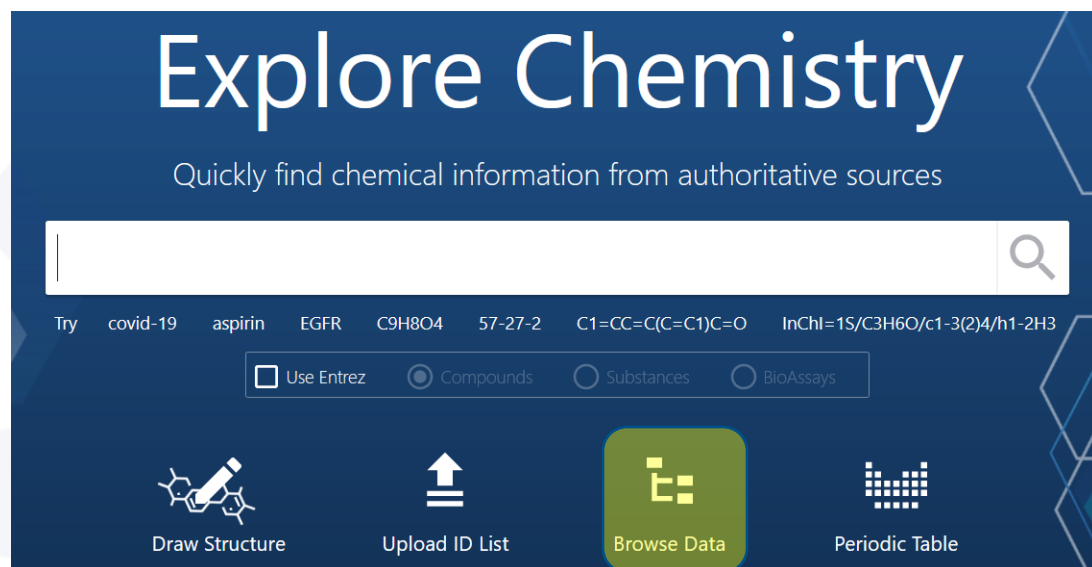
Create: 2004-09-16
Modify: 2023-08-12

Description

Toluene is a clear, colorless liquid with a distinctive smell. Toluene occurs naturally in crude oil and in the tolu tree. It is also produced in the process of making gasoline and other fuels from crude oil and making coke from coal. Toluene is used in making paints, paint thinners, fingernail polish, lacquers, adhesives, and rubber and in some printing and leather tanning processes.

► [Agency for Toxic Substances and Disease Registry \(ATSDR\)](#)

Hundreds of compound-specific annotations are available



The PubChem Compound TOC (Table of Contents) classification contains a browse-able tree of all available sections within PubChem Compound records.

Find records with a specific annotation

Click to expand

- PubChem Compound TOC ? 67,315,316
 - Agrochemical Information ? 3,147
 - Associated Disorders and Diseases ? 30,152
 - Biologic Description ? 2,509,996
 - Biological Test Results ? 4,566,405
 - Chemical and Physical Properties ? 269,054
 - Classification ? 22,946,443
 - Drug and Medication Information ? 21,094
 - Food Additives and Ingredients ? 7,706
 - Identification ? 4,873
 - Information Sources ? 47,695,668
 - Interactions and Pathways ? 206,660
 - Literature ? 4,075,481
 - Names and Identifiers ? 6,989,156
 - Patents ? 39,103,377
 - Pharmacology and Biochemistry ? 114,315
 - Related Records ? 13,273,055
 - Safety and Hazards ? 185,273
 - Spectral Information ? 1,576,030
 - Structures ? 11,818,832
 - Toxicity ? 118,258
 - Use and Manufacturing ? 108,235
- Chemical Safety ? 181,153
- Minerals ? 380
- Taxonomy ? 242,799

- Chemical and Physical Properties ? 269,054
 - Experimental Properties ? 245,101
 - Acid Value ? 20
 - Autoignition Temperature ? 954
 - Boiling Point ? 6,166
 - Caco2 Permeability ? 86
 - Chemical Classes ? 18,244
 - Collision Cross Section ? 6,564
 - Color/Form ? 6,264
 - Corrosivity ? 699
 - Decomposition ? 3,862
 - Density ? 5,873
 - Dielectric Constant ? 3
 - Dispersion ? 1
 - Dissociation Constants ? 2,608
 - Enthalpy of Sublimation ? 11
 - Flash Point ? 2,182
 - Heat of Combustion ? 532
 - Heat of Vaporization ? 714
 - Henry's Law Constant ? 3,260
 - Hydrophobicity ? 19
 - Ionization Efficiency ? 458
 - Ionization Potential ? 290
 - Isoelectric Point ? 29
 - Kovats Retention Index ? 70,656

SEARCH FOR

PubChem: PubChem Compound TOC: Flash Point

Treating this as a previously computed list of identifiers.

Compounds

2,182 results

Filters

SORT BY Relevance



1-Aminopropan-2-ol; 1-AMINO-2-PROPANOL; 78-96-6; Isopropanolamine; Amino-2-propanol; .

Compound CID: 4

MF: C₃H₉NO MW: 75.11g/mol

IUPAC Name: 1-aminopropan-2-ol

Isomeric SMILES: CC(CN)O

InChIKey: HXXKHQJGJAFBHI-UHFFFAOYSA-N

InChI: InChI=1S/C3H9NO/c1-3(5)2-4/h3,5H,2,4H2,1H3

Create Date: 2005-03-26

Summary

Similar Structures Search

Related Records



1-chloro-2,4-dinitrobenzene; 2,4-Dinitrochlorobenzene; 97-00-7; Dinitrochlorobenzene; DNCB; .

Compound CID: 6

MF: C₆H₃ClN₂O₄ MW: 202.55g/mol

IUPAC Name: 1-chloro-2,4-dinitrobenzene

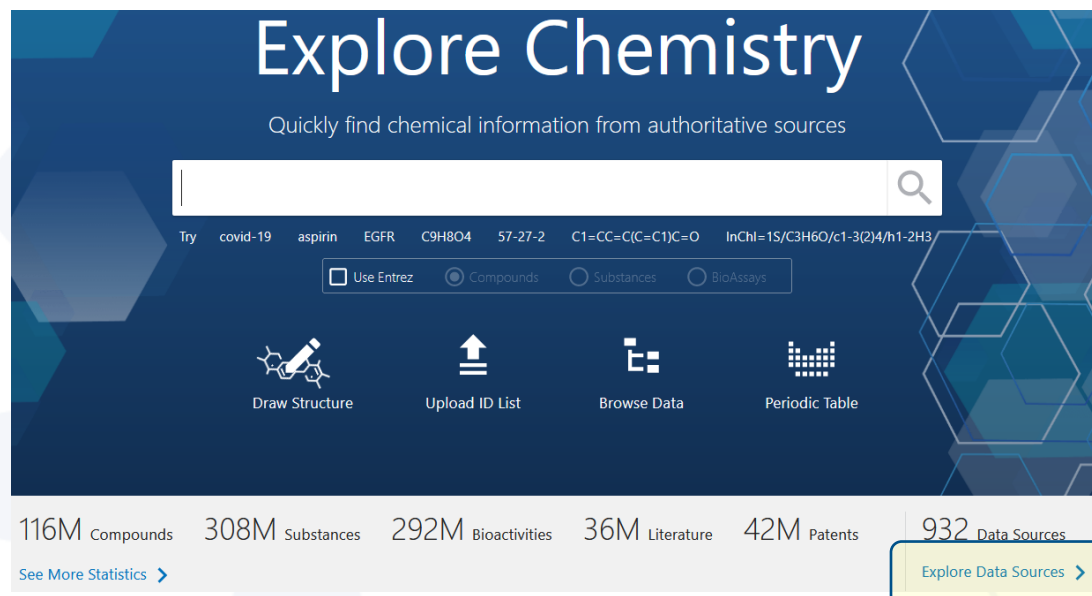
Isomeric SMILES: C1=CC(=C(C(=C1[N+](=O)[O-])[N+](=O)[O-])Cl

InChIKey: VYZAHLCBVHPDDF-UHFFFAOYSA-N

InChI: InChI=1S/C6H3ClN2O4/c7-5-2-1-4(8(10)11)3-6(5)9(12)13/h1-3H

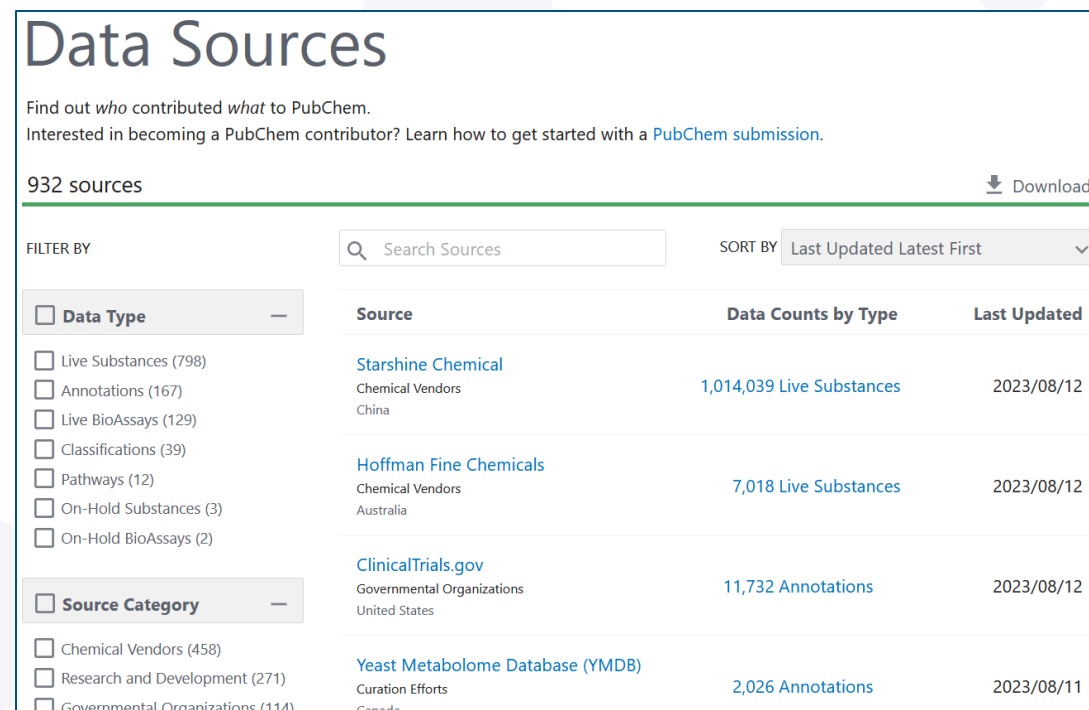
Create Date: 2005-03-26

Hundreds of data sources



The 'Explore Chemistry' interface features a dark blue header with the title 'Explore Chemistry' and the subtitle 'Quickly find chemical information from authoritative sources'. Below the header is a search bar and a row of tabs: 'Try', 'covid-19', 'aspirin', 'EGFR', 'C9H8O4', '57-27-2', 'C1=CC=C(C=C1)C=O', and 'InChI=1S/C3H6O/c1-3(2)4/h1-2H3'. A filter bar shows 'Use Entrez' (unchecked), 'Compounds' (selected), 'Substances' (unchecked), and 'BioAssays' (unchecked). Below the filter bar are four icons: 'Draw Structure', 'Upload ID List', 'Browse Data', and 'Periodic Table'. At the bottom, a statistics bar shows: '116M Compounds', '308M Substances', '292M Bioactivities', '36M Literature', '42M Patents', and '932 Data Sources'. A button labeled 'Explore Data Sources' is highlighted with a blue arrow pointing to the right.

The PubChem Data Sources interface contains a list of all available data sources within PubChem that one can search, filter, and download.



The 'Data Sources' interface has a title 'Data Sources' and a subtitle 'Find out who contributed what to PubChem. Interested in becoming a PubChem contributor? Learn how to get started with a [PubChem submission](#).' Below the subtitle is a '932 sources' header with a 'Download' button. A 'FILTER BY' section includes a search bar 'Search Sources' and a 'SORT BY' dropdown set to 'Last Updated Latest First'. The main content is a table with columns: 'Data Type', 'Source', 'Data Counts by Type', and 'Last Updated'.

Data Type	Source	Data Counts by Type	Last Updated
<input type="checkbox"/> Live Substances (798)	Starshine Chemical	1,014,039 Live Substances	2023/08/12
<input type="checkbox"/> Annotations (167)	Chemical Vendors China		
<input type="checkbox"/> Live BioAssays (129)	Hoffman Fine Chemicals	7,018 Live Substances	2023/08/12
<input type="checkbox"/> Classifications (39)	Chemical Vendors Australia		
<input type="checkbox"/> Pathways (12)	ClinicalTrials.gov	11,732 Annotations	2023/08/12
<input type="checkbox"/> On-Hold Substances (3)	Governmental Organizations United States		
<input type="checkbox"/> On-Hold BioAssays (2)	Yeast Metabolome Database (YMDB)	2,026 Annotations	2023/08/11
<input type="checkbox"/> Source Category	Curation Efforts Canada		
<input type="checkbox"/> Chemical Vendors (458)			
<input type="checkbox"/> Research and Development (271)			
<input type="checkbox"/> Governmental Organizations (114)			

Find data sources and what they provide

Data Sources

Find out *who* contributed *what* to PubChem.
Interested in becoming a PubChem contributor? Learn how to get started with a [PubChem submission](#).

80 sources [Download](#)

FILTER BY 2 active X

Search Sources

SORT BY Last Updated Latest First

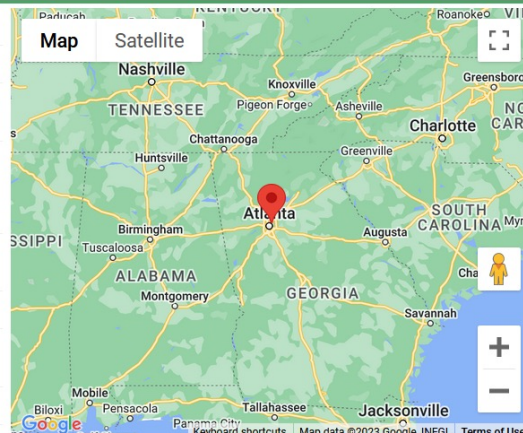
	Source	Data Counts by Type	Last Updated
<input checked="" type="checkbox"/> Data Type			
<input checked="" type="checkbox"/> Annotations (80)			
<input type="checkbox"/> Live Substances (39)			
<input type="checkbox"/> Classifications (19)			
<input type="checkbox"/> Live BioAssays (15)			
<input type="checkbox"/> On-Hold BioAssays (2)			
<input type="checkbox"/> Pathways (1)			
<input type="checkbox"/> On-Hold Substances (1)			
<input checked="" type="checkbox"/> Source Category			
<input checked="" type="checkbox"/> Governmental Organizations (80)			
<input type="checkbox"/> Curation Efforts (72)			
<input type="checkbox"/> Research and Development (42)			
<input type="checkbox"/> Journal Publishers (10)			
<input type="checkbox"/> Subscription Services (4)			
<input type="checkbox"/> NIH Initiatives (3)			
	ClinicalTrials.gov Governmental Organizations United States	11,732 Annotations	2023/08/12
	USGS National Minerals Information Center Governmental Organizations United States	94 Annotations	2023/08/11
	NLM RxNorm Terminology Governmental Organizations United States	6,896 Annotations	2023/08/11
	NIST Physical Measurement Laboratory Governmental Organizations United States	118 Annotations	2023/08/11
	NIOSH Manual of Analytical Methods Governmental Organizations United States	906 Annotations	2023/08/11

DATA SOURCES

NIOSH Manual of Analytical Methods

NIOSH Manual of Analytical Methods (NMAM) is a collection of methods for sampling and analysis of contaminants in workplace air, and in the blood and urine of workers who are occupationally exposed. These methods have been developed or adapted by NIOSH or its partners and have been evaluated according to established experimental protocols and performance criteria.

Organization	CDC
Category	Governmental Organizations
URL	https://www.cdc.gov/niosh/docs/2003-154/
License Note	The information provided using CDC Web site is only intended to be general summary information to the public. It is not intended to take the place of either the written law or regulations.
License URL	https://www.cdc.gov/Other/discclaimer.html
Contact Name	NIOSH CDC
Address	1600 Clifton Road, Atlanta, GA, United States, 30329-4027
Data Source ID	13124
Data in PubChem	906 Annotations
Last Updated	2023/08/11



DATA SOURCES > NIOSH MANUAL OF ANALYTICAL ... > ANNOTATIONS

Annotations from NIOSH Manual of Analytical Methods

1 annotation topic [Download](#)

906 total annotation data items

NIOSH Analytical Methods (Compound)	Download
-------------------------------------	--------------------------

Health and Safety data in PubChem

- More than 100 data sources provide health and safety, toxicity, and property data



Are we missing data sources that you use? What should be added?

Describing the indescribable (UVCBs)

COMPOUND SUMMARY

Asbestos

See also:  [Chrysotile Asbestos](#) (related);  [Crocidolite Asbestos](#) (related); [Tremolite Asbestos](#) (related)

[... View More ...](#)

PubChem CID	Not available because this is not a discrete structure.
Molecular Formula	[Mg ₆ (Si ₄ O ₁₀)(OH) ₈]
Description	<p>Asbestos is the name given to a group of six different fibrous minerals (amosite, chrysotile, crocidolite, and the fibrous varieties of tremolite, actinolite, and anthophyllite) that occur naturally in the environment. Asbestos minerals have separable long fibers that are strong and flexible enough to be spun and woven and are heat resistant. Because of these characteristics, asbestos has been used for a wide range of manufactured goods, mostly in building materials (roofing shingles, ceiling and floor tiles, paper products, and asbestos cement products), friction products (automobile clutch, brake, and transmission parts), heat-resistant fabrics, packaging, gaskets, and coatings. Some vermiculite or talc products may contain asbestos.New!</p> <p>► Agency for Toxic Substances and Disease Registry (ATSDR)</p>

PubChem Asbestos (Compound)

10 Safety and Hazards

10.1 Hazards Identification

10.1.1 GHS Classification

1 of 9

[View All](#)

Pictogram(s)



Health Hazard

Signal

Danger

GHS Hazard Statements

H350: May cause cancer [Danger Carcinogenicity]
H372 **: Causes damage to organs through prolonged or repeated exposure [Danger Specific target organ toxicity, repeated exposure]

Precautionary Statement Codes

P203, P260, P264, P270, P280, P318, P319, P405, and P501
(The corresponding statement to each P-code can be found at the [GHS Classification](#) page.)

► [EU REGULATION \(EC\) No 1272/2008](#)

10.1.2 Hazard Classes and Categories

Carc. 1A

STOT RE 1

► [EU REGULATION \(EC\) No 1272/2008](#)

Carc. 1A (100%)

► [European Chemicals Agency \(ECHA\)](#)

Describing the indescribable (UVCBs)

COMPOUND SUMMARY

Asbestos

See also:  [Chrysotile Asbestos](#) (related);  [Crocidolite Asbestos](#) (related); [Tremolite Asbestos](#) (related)



[... View More ...](#)

PubChem CID	Not available because this is not a discrete structure.
Molecular Formula	$[\text{Mg}_6(\text{Si}_4\text{O}_{10})(\text{OH})_8]$
Description	<p>Asbestos is the name given to a group of six different fibrous minerals (amosite, chrysotile, crocidolite, and the fibrous varieties of tremolite, actinolite, and anthophyllite) that occur naturally in the environment. Asbestos minerals have separable long fibers that are strong and flexible enough to be spun and woven and are heat resistant. Because of these characteristics, asbestos has been used for a wide range of manufactured goods, mostly in building materials (roofing shingles, ceiling and floor tiles, paper products, and asbestos cement products), friction products (automobile clutch, brake, and transmission parts), heat-resistant fabrics, packaging, gaskets, and coatings. Some vermiculite or talc products may contain asbestos. New!</p> <p>Agency for Toxic Substances and Disease Registry (ATSDR)</p>

PubChem Asbestos (Compound)

4 Related Records

4.1 Other Relationships

-  [Chrysotile Asbestos](#) (related)
-  [Crocidolite Asbestos](#) (related)
- [Tremolite Asbestos](#) (related)
- [Amosite Asbestos](#) (related)
- [Anthophyllite Asbestos](#) (related)
- [Actinolite Asbestos](#) (related)

[PubChem](#)

4.2 Associated Chemicals

Anthophyllite;17068-78-9

[Hazardous Substances Data Bank \(HSDB\)](#)

Actinolite;13768-00-8

[Hazardous Substances Data Bank \(HSDB\)](#)

Crocidolite;12001-28-4

[Hazardous Substances Data Bank \(HSDB\)](#)

Describing the indescribable (UVCBs)

Recently introduced, the PubChem Reference Collection includes a set of records that include undefined, variable, complex mixtures, and biologics. It also includes reference information from curated and authoritative data sources such as chemical structure and chemical names.

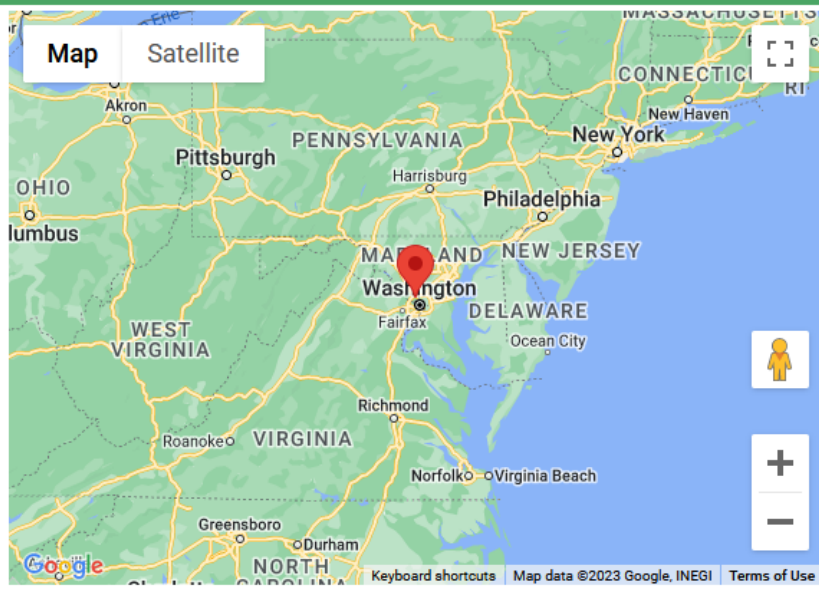
Internally, we call these substance records “concepts” and they help PubChem improve the quality of information.

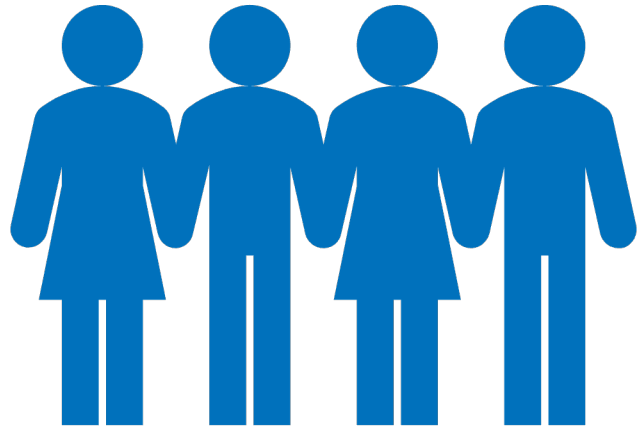
DATA SOURCES

PubChem Reference Collection

The PubChem Reference Collection contains a reference set of chemical substances derived from authoritative and curated data sources. These substances contain the chemical names and (when applicable) a representative chemical structure used by PubChem to link to chemical substance annotations. This collection includes structures that lack full atomic-level detail: polymers, complex mixtures, unknown or variable composition, biologics, reaction products, and more. The quality of this data set may be annotated as a comment relative to the availability of authoritative and curated data sources.

Organization	PubChem
Category	Governmental Organizations
URL	https://pubchem.ncbi.nlm.nih.gov/
Contact Name	PubChem Staff
Address	8600 Rockville Pike, Bethesda, MD, United States, 20894
Data Source ID	26136
Data in PubChem	53,547 Live Substances
Last Updated	2023/07/25

A map of the Washington, D.C. area, showing the location of the National Library of Medicine. The map includes labels for various cities and states, such as Washington, D.C., Maryland, Virginia, Pennsylvania, New Jersey, Delaware, and New York. A red pin is placed on the map near the National Library of Medicine. The map also shows major roads and water bodies. The map is titled 'Map' and 'Satellite'.



Engaging the community

Multi-year engagements with many parties involved

.. here are some examples



Engaging the community

- ACS Professional Divisions have been pivotal
- CINF (Leah McEwen) and CHAS (Ralph Stuart)
 - Answer key questions necessary for progress
 - What is needed and how to present it?
 - Provided a trajectory towards improvements
 - Use cases, content, and interfaces
 - ***PubChem LCSS and other engagements***

Laboratory Chemical Safety Summary (LCSS) views now available in PubChem

Posted on August 17, 2015

The PubChem Laboratory Chemical Safety Summary (LCSS) provides pertinent chemical health and safety data for a given PubChem Compound record. The PubChem LCSS is a community effort involving professionals in health and safety, chemistry librarianship, informatics, and other specialties.

What is LCSS?

The screenshot shows the PubChem website interface. At the top, there's a navigation bar with 'NIH', 'NLM', and 'National Center for Biotechnology Information'. Below this is the 'PubChem' logo and 'OPEN CHEMISTRY DATABASE'. A search bar is on the right. The main header is brown and says 'LCSS Laboratory Chemical Safety Summary for CID 1140'. Below this, there are links for 'Download', 'Print', 'Share', and 'Help'. The breadcrumb trail reads 'PUBCHEM > COMPOUND > TOLUENE > LCSS'. The title 'Toluene' is prominently displayed. To the right of the title is a 'Cite this Record' button. Below the title, there's a table with chemical data: PubChem CID: 1140, Chemical Names: Toluene; Methylbenzene; Toluol; Methylbenzol; Phenylmethane; Benzene, methyl-, Molecular Formula: C₇H₈, and Molecular Weight: 92.13842 g/mol. A 'Contents' section on the left lists: 1 GHS Classification, 2 Identifiers, 3 Physical Properties, 4 Toxicity Data, 5 Exposure Limits, 6 Health and Symptoms, and 7 First Aid. The '1 GHS Classification' section is expanded, showing three hazard pictograms (flame, health hazard, and exclamation mark) and a list of hazard statements: Signal: Dgr, H225 - Highly flammable liquid and vapour, H361d ***, H304 - May be fatal if swallowed and enters airways, and H373 **.



Engaging the community

Univ. California, CHAS, IUPAC, ...

- Series of meetings, workshops, and interactions
- Many practical issues to overcome
- Mixtures are very important
- MInChI, IUPAC InChI QR Codes, ...
- *Big influence on PubChem efforts*

Publicly Available Published by De Gruyter November 18, 2022

Specification of International Chemical Identifier (InChI) QR codes for linking labels on containers of chemical samples to digital resources (IUPAC Recommendations 2021)

Jeremy G. Frey, Richard M. Hartshorn and Leah R. McEwen

From the journal [Pure and Applied Chemistry](#)

<https://doi.org/10.1515/pac-2021-0604>

Cite this

Share this

Abstract

This article discusses the ways of linking physical objects to digital information relevant to chemical entities, specifically those that can be described by the use of the IUPAC International Chemical Identifier (InChI). It makes recommendations on the form of the computer readable components of labels provided for chemicals and materials that are used on product/sample containers and on the associated documentation that is used when transporting these containers (either internally or during export/import). The focus is on specification of the content of the 2D Quick Response bar codes required to describe the molecular content of the containers and link to digital resources to supplement that provided on a physical label. The necessary technical and (possible) business infrastructure necessary to support the use of the InChI and InChIKey for rapid recall of relevant information is considered here and suggestions are made.

Keywords: [cheminformatics](#); [InChI](#); [InChIKey](#); [International Chemical Identifier](#); [IUPAC](#); [QR code](#)



Engaging the community

Pistoia Alliance Chemical Safety Library, ...

- Chemical reaction safety importance
- Need for community-based resources for (unexpected) reactivity hazards
- *PubChem CAMEO Chemical Reactivity Classification integration*
- *Pistoia Alliance CSL data source*

https://safescience.cas.org/

Log In Create Account

Pistoia Alliance

The Pistoia Alliance Chemical Safety Library (CSL) provides unique chemical safety data to scientists to potential dangerous experiments. CAS, a division of the American Chemical Society, provided this open access platform to serve scientists worldwide.

Search by CAS Registry Number, CSL Number, Chemical Name, SMILES

Enter a query...

[Learn more about boolean searching in the Chemical Safety Library.](#)

DATA SOURCES

Pistoia Alliance Chemical Safety Library

The Pistoia Alliance is a global, not-for-profit member organization of chemical industry, government, publishers, and academic groups working to lower barriers to chemical safety data and foster collaboration. The Pistoia Chemical Safety Library is a freely accessible database of chemical safety data to foster chemical safety across academic and industrial laboratories.

Organization	Pistoia Alliance
Category	Research and Development
URL	https://www.pistoiaalliance.org/
License URL	https://www.cas.org/site/content/cas/en/files/documents/chemical-safety-library-terms.pdf
Contact Name	Gabrielle Whittick
Address	401 Edgewater Place, Suite 600, Wakefield, MA, United States, 01880
Data Source ID	22015
Data in PubChem	133 Annotations
Last Updated	2019/08/14

CAMEO Chemical Reactivity Classification 4,793

- ▶ Acetals, Ketals, Hemiacetals, and Hemiketals 194
- ▶ Acids, Carboxylic 40
- ▶ Acids, Strong Non-oxidizing 25
- ▶ Acids, Strong Oxidizing 96
- ▶ Acids, Weak 53
- ▶ Acrylates and Acrylic Acids 613
- ▶ Acyl Halides, Sulfonyl Halides, and Chloroformates
- ▶ Alcohols and Polyols 73
- ▶ Aldehydes 10
- ▶ Alkynes, with Acetylenic Hydrogen 8
- ▶ Alkynes, with No Acetylenic Hydrogen 409
- ▶ Amides and Imides 293
- ▶ Amines, Aromatic 722
- ▶ Amines, Phosphines, and Pyridines 30
- ▶ Anhydrides 360
- ▶ Aryl Halides 48
- ▶ Azo, Diazo, Azido, Hydrazine, and Azide Compounds 27
- ▶ Bases, Strong 69
- ▶ Bases, Weak 15
- ▶ Carbamates 34
- ▶ Carbonate Salts
- ▶ Chlorosilanes



Engaging the community

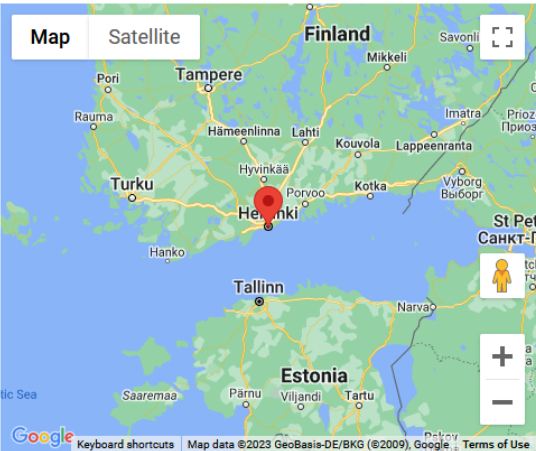
European Chemicals Agency (ECHA), CHAS, ...

- Difficulties disseminating REACH data
- Programmatic access tools (APIs)
- Primary source of GHS information
- How to summarize many GHS reports?
- Improved PubChem GHS displays, classification

European Chemicals Agency (ECHA)

The European Chemicals Agency (ECHA) is the driving force among regulatory authorities in implementing the EU's groundbreaking chemicals legislation for the benefit of human health and the environment as well as for innovation and competitiveness.

Organization	European Chemicals Agency
Category	Governmental Organizations
URL	https://echa.europa.eu/
License Note	Use of the information, documents and data from the ECHA website is subject to the terms and conditions of this Legal Notice, and subject to other binding limitations provided for under applicable law, the information, documents and data made available on the ECHA website may be reproduced, distributed and/or used, totally or in part, for non-commercial purposes provided that ECHA is acknowledged as the source: "Source: European Chemicals Agency, http://echa.europa.eu/ ". Such acknowledgement must be included in each copy of the material. ECHA permits and encourages organisations and individuals to create links to the ECHA website under the following cumulative conditions: Links can only be made to webpages that provide a link to the Legal Notice page.
License URL	https://echa.europa.eu/web/guest/legal-notice








H225 (98.41%): Highly Flammable liquid and vapor [Danger Flammable liquids]
H304 (99.92%): May be fatal if swallowed and enters airways [Danger Aspiration hazard]
H315 (98.42%): Causes skin irritation [Warning Skin corrosion/irritation]
H336 (100%): May cause drowsiness or dizziness [Warning Specific target organ toxicity, single effects]
H361 (98.51%): Suspected of damaging fertility or the unborn child [Warning Reproductive toxicity]
H373 (100%): Causes damage to organs through prolonged or repeated exposure [Warning Organ toxicity, repeated exposure]

5 annotation topics

 Download

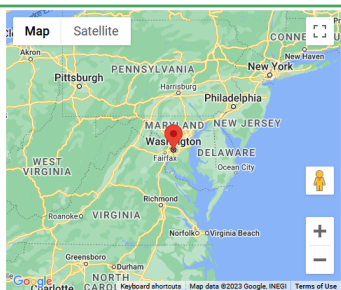
496,704 total annotation data items

CAS (Compound)	 Download
European Community (EC) Number (Compound)	 Download
GHS Classification (Compound)	 Download
Hazard Classes and Categories (Compound)	 Download
Highly Hazardous Substance (Compound)	 Download

EPA Substance Registry Services

The US EPA catalogs the substances (chemicals, biological organisms, properties) that are tracked or regulated at EPA. SRS identifies which EPA program or state or tribal program manages the substance and by which synonym.

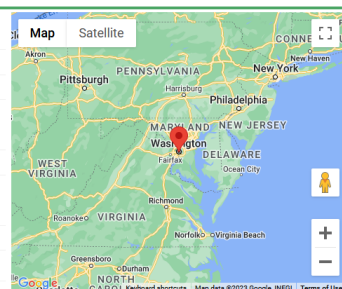
Organization	US EPA
Category	Governmental Organizations
URL	https://ofmpub.epa.gov/sor_internet/registry/substreg/landingPage.do
License URL	https://www.epa.gov/privacy/policy-act-laws-policies-and-re-sources
Contact Name	Akshay Narang
Address	1301 Pennsylvania Ave NW, Washington, DC, United States, 20460
Data Source ID	2331
Data in PubChem	115,032 Live Substances 1 Classification
Last Updated	2022/07/13



EPA Pesticide Ecotoxicity Database

The Ecological Fate and Effects Division of the US EPA Office of Pesticide Programs provide ecotoxicity endpoints for pesticides registered or previously registered in the U.S. Toxicity data on over 4,000 active ingredients, metabolites, and multi-ingredient formulations. The toxicity data is compiled from actual studies reviewed by EPA in conjunction with pesticide registration or re-registration and studies performed by US EPA, USDA and US FWS laboratories which have been reviewed by Agency biologists and judged acceptable for use in the ecological risk assessment process.

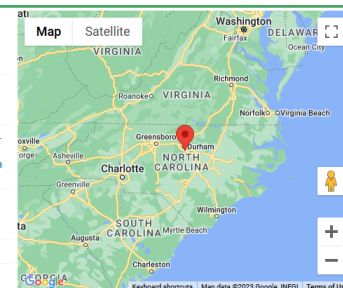
Organization	US Environmental Protection Agency - EPA
Category	Governmental Organizations
URL	https://ecotox.ipmcenters.org/
License URL	https://www.epa.gov/privacy/policy-act-laws-policies-and-re-sources
Contact Name	EPA OPP Staff
Address	1200 Pennsylvania Ave, N.W., Washington, DC, United States, 20460
Data Source ID	15219
Data in PubChem	1,253 Annotations
Last Updated	2023/08/11



EPA DSSTox

The U.S. EPA Distributed Structure-Searchable Toxicity (DSSTox) Database provides a high quality public chemistry resource for supporting improved predictive toxicology. A distinguishing feature of this effort is the accurate mapping of bioassay and physicochemical property data associated with chemical substances to their corresponding chemical structures.

Organization	National Center for Computational Toxicology (NCCT) Office of Research and Development, US EPA
Category	Research and Development, Governmental Organizations, Curation Efforts
URL	https://www.epa.gov/chemical-research/distributed-structure-searchable-toxicity-dssto-data-base
License URL	https://www.epa.gov/privacy/policy-act-laws-policies-and-re-sources
Contact Name	Ann Richard
Address	Mail Drop D343-03, Research Triangle Park, NC, United States, 27711
Data Source ID	EPA DSSTox
Data in PubChem	1,235,318 Live Substances 12 Live BioAssays 1,217,621 Annotations 1 Classification
Last Updated	2023/05/17



NORMAN Suspect List Exchange

The NORMAN network enhances the exchange of information on emerging environmental substances, and encourages the validation and harmonisation of common measurement methods and monitoring tools so that the requirements of risk assessors and risk managers can be better met. The NORMAN Suspect List Exchange (NORMAN-SLE) is a central access point to find suspect lists relevant for various environmental monitoring questions, described in DOI:10.1186/s12302-022-00680-6

Organization	NORMAN Network (c/o Unilu)
Category	Research and Development
URL	https://www.norman-network.com/nds/SLE/
License Note	Data: CC-BY 4.0; Code (hosted by ECL): CC-BY 4.0; Artistic: 2.0
License URL	https://creativecommons.org/licenses/by/4.0/
Contact Name	Emma Schymanski
Address	6 avenue du Swing, Belvaux, Luxembourg, 4367
Data Source ID	23819
Data in PubChem	118,487 Live Substances 22,355 Annotations 1 Classification
Last Updated	2023/08/11



DATA SOURCES > NORMAN SUSPECT LIST EXCHANGE > CLASSIFICATIONS

Classifications from NORMAN Suspect List Exchange

1 classification

NORMAN Suspect List Exchange Classification

The NORMAN Suspect List Exchange (NORMAN-SLE) is a central access point for NORMAN members (and others) to find suspect lists relevant for their environmental monitoring questions.

Update: 2023-08-08 18:00:01

This Exchange documents all individual collections that (will) form a part of NORMAN SusDat, the merged NORMAN Substance Database (DOI:10.5281/zenodo.2664077). Each list/collection has a DOI in Zenodo.

<https://www.norman-network.com/nds/SLE/>



Engaging the community

Environmental Protection Agency (EPA), Norman SLE, ...

- Chemical information is highly nuanced
- Regulatory needs can be different
- Many new data sources and improved integration
- Describing the “indescribable” (UVCBs)
- *PubChem “concept” infrastructure introduced*



Engaging the community

Chemical Abstract Services, EPA, IUPAC, ...


- Improving the quality and trust of information
- Clarifying CAS Registry Number and chemical structure associations
- Scoping of “common” chemicals
- *Revamp of the CAS Common Chemistry website*

CAS Common Chemistry

CAS Common Chemistry is an open community resource for accessing chemical information. Nearly 500,000 chemical substances from CAS REGISTRY cover areas of community interest, including common and frequently regulated chemicals, and those relevant to high school and undergraduate chemistry classes. This chemical information, curated by our expert scientists, is provided in alignment with our mission as a division of the American Chemical Society.


Organization	CAS
Category	Subscription Services
URL	https://commonchemistry.cas.org/
License Note	The data from CAS Common Chemistry is provided under a CC-BY-NC 4.0 license, unless otherwise stated.
License URL	https://creativecommons.org/licenses/by-nc/4.0/
Contact Name	CAS Common Chemistry
Address	2540 Olentangy River Road, Columbus, Ohio, United States, 43210
Data Source ID	24603
Data in PubChem	428,590 Annotations
Last Updated	2021/05/12



 Common Chemistry

About CASContact

Search by chemical compound name, SMILES, InChI or CAS Registry Number® (CAS RN®)

Enter a query...

e.g. aspirin, sodium chloride, 58-08-2, C=O

CAS Common Chemistry is an open community resource for accessing chemical information. Nearly 500,000 chemical substances from CAS REGISTRY® cover areas of community interest, including common and frequently regulated chemicals, and those relevant to high school and undergraduate chemistry classes. This chemical information, curated by our expert scientists, is provided in alignment with our mission as a division of the American Chemical Society.

Access Common Chemistry via API

Access the CAS Common Chemistry chemical database via API (application programming interface) to support workflow integration, chemical research and cheminformatics.

Full access to the CAS content collection is available through custom data and analytics solutions or in CAS products such as SciFinder® and STNNext®.

<https://commonchemistry.cas.org/>

CAS Common Chemistry is provided under the [Creative Commons Attribution-NonCommercial 4.0 International License](#), or CC BY-NC 4.0 license. By using CAS Common Chemistry, you agree to the terms and conditions of this license. To use or license CAS Common Chemistry for commercial purposes, [contact us](#).

Summing it all up



Community
engagements are
key

Heavily influence
changes made to
PubChem



It is all about the
use cases

What does the
community need?
Why does the
community need
it?



PubChem is your
safety resource

How can we help?

PubChem Crew ...

Evan Bolton

Jie Chen

Tiejun Cheng

Asta Gindulyte

Jane He

Siqian He

Sunghwan Kim

Qingliang Li

Ben Shoemaker

Paul Thiessen

Bo Yu

Leonid Zaslavsky

Jian Zhang

Special thanks to the NCBI Help Desk, the NCBI Systems teams, and past PubChem group members

Special thanks

- All PubChem contributors and collaborators
- Health and Safety collaborators (especially Ralph Stuart, Leah McEwen)
- Exposomics collaborators (especially Emma Schymanski, NORMAN SLE)
- IUPAC collaborators (especially InChI contributors, Leah McEwen)
- Software collaborators
 - NextMove Software (Roger Sayle, John May) and Daniel Lowe / Noel O'Boyle
 - Xemistry GmbH (Wolf D. Ihlenfeldt)
 - OpenEye Scientific Software
- This research was supported by the National Center for Biotechnology Information (NCBI) of the National Library of Medicine (NLM), National Institutes of Health (NIH)

Improve interpretation

the world is a small place

Help identify and close knowledge gaps

use cases, use cases, use cases

Science
is data
driven

Open science is grand ...



Bring your data into the light

*... so others can build off it and
advance the (data) science*

making data FAIR

many data gaps

Information in
the public
domain helps
everybody

Increase the utility of your research

many hands make light work

Support interpretation of complex data

more data is more data

open science infrastructure is here and now

