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Chemical Safety and Hazard Information in PubChem

Jian Zhang*, Paul Thiessen, Asta Gindulyte, Leah McEwen, Ralph Stuart,
Evan Bolton, Steve Bryant

National Center for Biotechnology Information

National Library of Medicine

National Institutes of Health

U.S. Department of Health and Human Services

Background

Chemical safety is a very important topic in chemical industry, academic labs, and even in our daily lives. It contains many aspects of scientific knowledge and technical components such as chemical property information, toxicity and ecological data, exposure and risk assessment information, and more detailed knowledge regarding environment and human health. Despite a lot of efforts, accidents still happen from time to time.

In the past few years, PubChem, an open source chemical information-hub, has integrated a lot of safety and hazard information into PubChem's annotation database. These information can be accessed through PubChem's web sites and services.



U.S. National Library of Medicine



Lab Accidents

The image is a screenshot of a web browser displaying a news article on the Chemistry World website. The browser's address bar shows the URL: www.rsc.org/chemistryworld/2016/01/tsinghua-university-postdoc-death-accident-chinese-lab-safety. The Chemistry World logo is prominently displayed at the top, along with navigation links for SHOP, BLOG, and REGISTER. The article title is "Deadly accident sounds alarm for safety in Chinese labs", dated 18 January 2016, by Hepeng Jia. The text describes a lab blast at Tsinghua University that resulted in the death of a postdoc researcher, raising concerns about lab safety in China. A photograph of a modern building, presumably the lab, is shown below the text. To the right of the article is an advertisement for Hiden Analytical's QGA Gas Analyser. Below the advertisement is a section titled "Related Content" featuring a link to a story about a lab explosion at Hawaii University. The browser's sidebar on the left shows a list of stories and a search bar.

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Deadly accident sounds alarm for safety in Chinese labs

18 January 2016 Hepeng Jia

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The lab blast that killed one postdoc researcher at [Tsinghua University](#) in late December has raised widespread safety concerns among Chinese chemists. They say a systematic reshuffle on lab safety is needed at Chinese research institutions. 'The bloody accident reflects a systematic negligence of safety in our labs,' says [Luo Min](#), a chemistry professor at [Ningxia University](#) located in the north-western Chinese city of Yinchuan.

The Beacon Photo: Kristy

Two 10th-g morning w burns.

HIDEN ANALYTICAL

QGA Gas Analyser

- ▶ Benchtop Compact System
- ▶ High Sensitivity - Wide Dynamic Range
- ▶ Zero Retention Time
- ▶ Real Time Trend Analysis
- ▶ Free iPad App

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www.HidenAnalytical.com

Related Content

California lab safety centre to investigate Hawaii University accident

13 April 2016 News and Analysis

Probe into recent lab explosion that took postdoc's arm to report at the end of April

Chemical Safety Information



U.S. National Library of Medicine



Chemical Safety Information Online

NIH NLM U.S. National Library of Medicine NCBI National Center for Biotechnology Information

PubChem | OPEN CHEMISTRY DATABASE

Search Compounds

About the Laboratory Chemical Safety Summary (LCSS) in PubChem

The Laboratory Chemical Safety Summary (LCSS) is based on the format described by the National Research Council in the publication "Prudent Practices in the Laboratory: Handling and Management of Chemical Hazards" (2011) (see reference below). The LCSS in PubChem contains pertinent chemical hazard and safety information. It is available when a GHS Classification ([Globally Harmonized System of Classification and Labeling of Chemicals](#)) is present for a given PubChem Compound record. The GHS classification codes and hazard pictograms are summarized in the [PubChem GHS page](#).

The LCSS provided by PubChem is intended to augment, not replace, safe laboratory practices and procedures for chemical information, such as those found in chemical inventory management systems or laboratory-specific personal protective equipment information. It is the responsibility of PubChem users to determine applicability of or gaps in the LCSS information to support safe use of a chemical. In addition, laboratory risks can arise not only from the specific chemicals used, but also from 1) changes in the concentrations and quantities of those chemicals, 2) new chemicals that are produced, 3) energy sources that occur during a laboratory process, and other variables. For more information, see [this newsletter article](#) as well as this [PubChem Blog post](#).

The electronic form of the LCSS provided by PubChem is publicly accessible. LCSS data can be downloaded as a data stream [in bulk](#) or on-demand from the PubChem website (e.g., by following a link on a compound summary page). Although we are not aware of any limitations or restrictions on the reuse of PubChem LCSS data, we are not able to give unconditional permission for reuse and advise consultation with intellectual property experts when reusing this data. See disclaimer below for more information.

Examples

- [Acetone](#)
- [Benzene](#)
- [Ethanol](#)
- [Formaldehyde](#)
- [Hydrogen Cyanide](#)
- [Imidazole](#)
- [Phenolphthalein](#)
- [Phosphoric Acid](#)
- [Theophylline](#)
- [Toluene](#)

[See a list of all compounds with LCSS](#)

References

PubChem Integrated Safety and Hazard Information from 20+ Sources



PubChem Overview

- ... public repository for chemical information.
- ... three linked databases - Substance, Compound, and BioAssay
- ... annotation database for experimental properties, drug and food chemical data, safety information, patents, literature, classifications...

PubChem Overview

- ... provides many services: web display, search system, data download, web services, widgets...
- .. Links, a lot of links to other NCBI database such as protein, gene, pubmed... and links to the original data pages.
- ... more to come ..

PubChem - where

- Google “pubchem”
- <https://pubchem.ncbi.nlm.nih.gov/>



PubChem Homepage

The PubChem Project

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

Databases >

Compounds:	91,671,620
Substances:	223,116,675
BioAssays:	1,218,668
Tested Compounds:	2,276,278
Tested Substances:	3,566,030
RNAi BioAssays:	91
BioActivities:	230,635,944
Protein Targets:	10,182
Gene Targets:	19,779

more ...

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PubChem Content

- **Compound summary** – unique structure information: 2d and 3d images, property data, drug, food additive, chemical safety, agrochemical, literature references, patents, and more – [PubChem most used information](#).
- **Annotations** – chemical annotation information from depositors and open sources.
- **Substance record** – depositor provided substance and related information.
- **BioAssay record** – depositor provided screening data and related information.

PubChem Compound Content

- 2D Structure
- 3D Conformer
- Biologic Description
- Names and Identifiers
- Chemical and Physical Properties
- Related Records
- Chemical Vendors
- Drug and Medication Information
- Food Additives and Ingredients
- Agrochemical Information
- Pharmacology and Biochemistry
- Use and Manufacturing
- Identification
- Safety and Hazards
- Toxicity
- Literature
- Patents
- Preparation and Reactions
- Biomolecular Interactions and Pathways
- Biological Test Results
- Classification

Safety and Hazard Information

- 2D Structure
- 3D Conformer
- Biologic Description
- Names and Identifiers
- Chemical and Physical Properties
- Related Records
- Chemical Vendors
- Drug and Medication Information
- Food Additives and Ingredients
- Agrochemical Information
- Pharmacology and Biochemistry
- Use and Manufacturing
- Identification
- Safety and Hazards
- Toxicity
- Literature
- Patents
- Preparation and Reactions
- Biomolecular Interactions and Pathways
- Biological Test Results
- Classification

Safety and Hazard Information

Safety and Hazards	Fire First Aid	REL-STEL	Reactivities and Incompatibilities
Hazards Identification	Explosion First Aid	REL-C	Transport Information
GHS Classification	Exposure First Aid	IDLH	DOT Emergency Guidelines
CLP Hazard Class and Category Codes	Inhalation First Aid	Conversion	Shipment Methods and Regulations
Health Hazard	Skin First Aid	Threshold Limit Values	DOT ID and Guide
Fire Hazard	Eye First Aid	Other Occupational Permissible Levels	DOT Label
Explosion Hazard	Ingestion First Aid	Sources and Potential Exposure	Packaging and Labelling
Hazards Summary	Fire Fighting Measures	Assessing Personal Exposure	EC Classification
Fire Potential	Fire Fighting	Occupational Exposure Limits	UN Classification
Skin, Eye, and Respiratory Irritations	Explosion Fire Fighting	Inhalation Risk	Emergency Response
Safety and Hazard Properties	Other Fire Fighting Hazards	Effects of Short Term Exposure	Regulatory Information
LEL	Accidental Release Measures	Effects of Long Term Exposure	DOT Emergency Response Guide
UEL	TIHGas	Radiation Limits and Potential	Isolation Name
Flammability	Isolation and Evacuation	Acceptable Daily Intakes	Isolation Distance
Critical Temperature	Spillage Disposal	Allowable Tolerances	Atmospheric Standards
Critical Pressure	Cleanup Methods	Personal Protection	Soil Standards
Danger of Explosion	Disposal Methods	Respirator Recommendations	Federal Drinking Water Standards
NFPA Hazard Classification	Other Preventative Measures	Fire Prevention	Federal Drinking Water Guidelines
NFPA Fire Rating	Handling and Storage	Explosion Prevention	State Drinking Water Standards
NFPA Reactivity Rating	Nonfire Spill Response	Exposure Prevention	State Drinking Water Guidelines
NFPA Health Rating	Safe Storage	Inhalation Prevention	Clean Water Act Requirements
NFPA Other	Storage Conditions	Skin Prevention	CERCLA Reportable Quantities
Physical Dangers	Exposure Control and Personal	Eye Prevention	TSCA Requirements
Chemical Dangers	Protection	Ingestion Prevention	RCRA Requirements
Explosive Limits and Potential	REL	Protective Equipment and Clothing	FIFRA Requirements
OSHA Standards	PEL	Stability and Reactivity	FDA Requirements
NIOSH Recommendations	PEL-TWA	Air and Water Reactions	Other Safety Information
Other Safety and Hazard Data	PEL-STEL	Reactive Group	Safety References
First Aid Measures	PEL-C	Reactivity Alerts	Safety Notes
First Aid	REL-TWA	Reactivity Profile	Toxic Combustion Products

Hazard Communication Safety Data Sheets

The Hazard Communication Standard (HCS) requires chemical manufacturers, distributors, or importers to provide Safety Data Sheets (SDSs) (formerly known as Material Safety Data Sheets or MSDSs) to communicate the hazards of hazardous chemical products. As of June 1, 2015, the HCS will require new SDSs to be in a uniform format, and include the section numbers, the headings, and associated information under the headings below:

Section 1, Identification includes product identifier; manufacturer or distributor name, address, phone number; emergency phone number; recommended use; restrictions on use.

Section 2, Hazard(s) identification includes all hazards regarding the chemical; required label elements.

Section 3, Composition/information on ingredients includes information on chemical ingredients; trade secret claims.

Section 4, First-aid measures includes important symptoms/effects, acute, delayed; required treatment.

Section 5, Fire-fighting measures lists suitable extinguishing techniques, equipment; chemical hazards from fire.

Section 6, Accidental release measures lists emergency procedures; protective equipment; proper methods of containment and cleanup.

Section 7, Handling and storage lists precautions for safe handling and storage, including incompatibilities.

Section 8, Exposure controls/personal protection lists OSHA's Permissible Exposure Limits (PELs); ACGIH Threshold Limit Values (TLVs); and any other exposure limit used or recommended by the chemical manufacturer, importer, or employer preparing the SDS where available as well as appropriate engineering controls; personal protective equipment (PPE).

Section 9, Physical and chemical properties lists the chemical's characteristics.

Section 10, Stability and reactivity lists chemical stability and possibility of hazardous reactions.

Section 11, Toxicological information includes routes of exposure; related symptoms, acute and chronic effects; numerical measures of toxicity.

Section 12, Ecological information*

Section 13, Disposal considerations*

Section 14, Transport information*

Section 15, Regulatory information*

Section 16, Other information, includes the date of preparation or last revision.

*Note: Since other Agencies regulate this information, OSHA will not be enforcing Sections 12 through 15 (29 CFR 1910.1200(g)(2)).



Safety and Hazard Information

PubChem integrated safety and hazard information from ~20 open source domains, and provided source links to allow users to be able to navigate to the original information page.

PubChem Safety and Hazard Information Sources



PubChem Safety and Hazard Information Sources

- ILO – ICSC
- OSHA Occupational Chemical Database
- NIOSH Pocket Guide to Chemical Hazards
- CAMEO Chemicals Database of Hazardous Materials
- HSDB
- EU REGULATION (EC) No 1272/2008
- Safe Work Australia - Hazardous Substances Information System (HSIS)
- Japanese NITE - Chemical Management Center (CMC)
- More ...

Where to find the Information

- Get safety and hazard information for a given chemical
- Get all compounds that have safety and hazard annotations
- Retrieve safety and hazard information programmatically

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Where to find the safety Information for a given chemical in pubChem

- Google
- PubChem homepage
- NCBI entrez PubChem compound
- Structure search
- Direct URL
- Other search engines: Bing, Yahoo, Baidu...

Case study: toluene: from Google

The screenshot shows a Google search interface with the query "toluene pubchem" entered in the search bar. The search results page displays "About 56,300 results (0.29 seconds)". The top result is "toluene | C₆H₅CH₃ - PubChem" with a link to <https://pubchem.ncbi.nlm.nih.gov/compound/toluene>. Below this, a brief description states: "Toluene is added to gasoline, used to produce benzene, and used as a solvent. Exposure to toluene may occur from breathing ambient or indoor air affected by ...". Key data points are listed: PubChem CID: 1140, Molecular Weight: 92.13842 g/mol, and Chemical Names: Toluene; Methylbenz... Molecular Formula: C₆H₅CH₃ or C₇H₈. Below the main result, several related compounds are listed in a grid:

TOLUENE-D8 TOLUENE-D8 C ₇ H ₈ CID 74861 - structure, chemical names ...	Dibenzyl toluene Dibenzyl toluene C ₂₁ H ₂₀ CID 3034397 - structure, chemical ...
4-Ethyltoluene 4-Ethyltoluene C ₉ H ₁₂ CID 12160 - structure, chemical ...	P-TOLUENESULFONAMIDE P-TOLUENESULFONAMIDE C ₇ H ₉ NO ₂ S CID 6269 ...
TOLUENE-3,4-DITHIOL TOLUENE-3,4-DITHIOL C ₇ H ₈ S ₂ CID 10334 - structure ...	2-Chlorotoluene 2-Chlorotoluene C ₆ H ₄ CH ₃ or CH ₃ C ₆ H ₄ Cl or C ₇ H ₇ Cl CID ...

More results from nih.gov »

Below the grid, another result is shown: "hydride toluene | C₇H₉- - PubChem" with a link to <https://pubchem.ncbi.nlm.nih.gov/compound/86595848>. The description for this result is: "hydride toluene | C₇H₉- | CID 86595848 - structure, chemical names, physical and chemical properties, classification, patents, literature, biological activities, ...". At the bottom, a partial result for "benzoyl peroxide toluene | C₂₁H₁₈O₄ - PubChem" is visible.

NIH

NCBI

Case study: toluene: from PubChem/Entrez

toluene - PubChem Compound

https://www.ncbi.nlm.nih.gov/pccompound/?term=toluene

NCBI Resources How To Sign in to NCBI

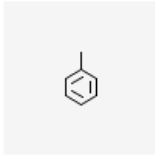
PubChem Compound PubChem Compound toluene Search Create alert Limits Advanced Help

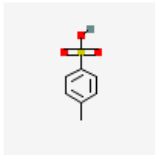
Summary 20 per page Sort by Default order Send to: Filters: Manage Filters

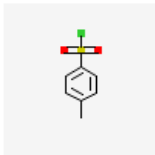
Search results

Items: 1 to 20 of 10493

<< First < Prev Page 1 of 525 Next > Last >>





- 

[toluene; methylbenzene; toluol ...](#)
MW: 92.138420 g/mol MF: C₇H₈
IUPAC name: **toluene**
Create Date: 2004-09-16
CID: 1140
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#) [PubMed](#)
[\(MeSH Keyword\)](#) [Active in 7 of 349 BioAssays](#)
- 

[P-TOLUENESULFONIC ACID; 4-Methylbenzenesulfonic acid; 104-15-4 ...](#)
MW: 172.201620 g/mol MF: C₇H₈O₃S
IUPAC name: 4-methylbenzenesulfonic acid
Create Date: 2005-03-26
CID: 6101
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#) [PubMed](#)
[\(MeSH Keyword\)](#) [Tested in 129 BioAssays](#)
- 

[Tosyl chloride; P-TOLUENESULFONYL CHLORIDE; 98-59-9 ...](#)
MW: 190.647280 g/mol MF: C₇H₇ClO₂S
IUPAC name: 4-methylbenzenesulfonyl chloride
Create Date: 2005-03-26
CID: 7397
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#) [PubMed](#)
[\(MeSH Keyword\)](#) [Tested in 1 BioAssay](#)

Actions on your results

-  **BioActivity Analysis**
Analyze the BioActivities of the compounds
-  **Structure Clustering**
Cluster structures based on structural similarity
-  **Structure Download**
Download the structures in various formats
-  **Pathways**
Analyze pathways containing the compounds

Refine your results

What's this?

Chemical Properties

Rule of 5 (4,989)

BioActivity Experiments

- BioAssays, Probes (1)
- BioAssays, Active (953)
- BioAssays, Tested (1,760)
- Protein 3D Structures (36)
- Crystal Structure Of Oxy-Human Hemoglobin Bassett At 2.15 Angstrom (1)
- Crystal Structure Of Sh2 In Complex With Ru78791 (1)
- Crystal Structure Analysis Of The Fkbp12 Complexed With 000308 Small Molecule (1)

NIH NCBI

Direct URL

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

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

<https://pubchem.ncbi.nlm.nih.gov/compound/1140>

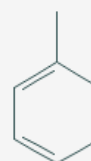
<https://pubchem.ncbi.nlm.nih.gov/compound/toluene>

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- 2 3D Conformer
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- 12 Safety and Hazards
- 13 Toxicity
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- 15 Patents
- 16 Biomolecular Interactions and Pathways
- 17 Biological Test Results
- 18 Classification
- 19 Information Sources

1 2D Structure

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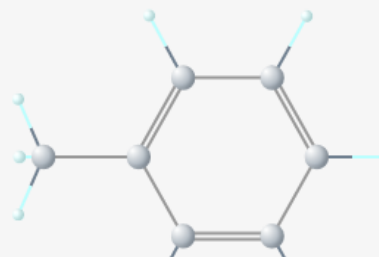


Magnify

from PubChem

2 3D Conformer

Search Download Get Image



toluene | C6H5CH3 - PubCh X

https://pubchem.ncbi.nlm.nih.gov/compound/toluene#section=Other-Identifiers

Compound Summary for CID 1140

Download Print Share Help

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 - 4.2.2 Color
 - 4.2.3 Odor
 - 4.2.4 Boiling Point

3.3 Other Identifiers

3.3.1 CAS

108-88-3

from ILO-ICSC, NIOSH-PocketGuide, OSHA Occupational Chemical DB, EPA Chemicals under the TSCA, ...

3.3.2 EC Number

203-625-9

from ECHA

3.3.3 ICSC Number

0078

from ILO-ICSC

3.3.4 RTECS Number

XS5250000

from ILO-ICSC, NIOSH-PocketGuide

3.3.5 UN Number

1294

from ILO-ICSC, OSHA Occupational Chemical DB, NJDOH RTK Hazardous Substance List, CAMEO Chemi...

1294

from Emergency Response Guidebook

3.3.6 UNII

3FPU23BG52

from FDA/SPL Indexing Data

toluene | C6H5CH3 - PubCh x

https://pubchem.ncbi.nlm.nih.gov/compound/toluene#section=Odor

Compound Summary for CID 1140

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 - 4.2.8 Density
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 - 4.2.10 Vapor Pressure
 - 4.2.11 LogP
 - 4.2.12 Auto-Ignition
 - 4.2.13 Decomposition
 - 4.2.14 Viscosity
 - 4.2.15 Corrosivity
 - 4.2.16 Heat of Combustion
 - 4.2.17 Heat of Vaporization
 - 4.2.18 Surface Tension
 - 4.2.19 Ionization Potential
 - 4.2.20 Odor Threshold
 - 4.2.21 Kovats Retention Index
 - 4.2.22 Chemical Classes
 - 4.3 Crystal Structures
 - 4.4 Spectral Properties

4.2.3 Odor

Sweet, pungent, benzene-like odor.

NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 310

from HSDB

4.2.4 Boiling Point

110.6 deg C

Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 79th ed. Boca Raton, FL: CRC Press Inc., 1998-1999., p. 3-55

from HSDB

111°C

from ILO-ICSC

232°F

from NIOSH-PocketGuide, OSHA Occupational Chemical DB

231.1° F at 760.0 mm Hg (NTP, 1992)

from CAMEO Chemicals

4.2.5 Melting Point

-94.9 deg C

Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 79th ed. Boca Raton, FL: CRC Press Inc., 1998-1999., p. 3-55

from HSDB

-95°C

from ILO-ICSC

-139°F

from NIOSH-PocketGuide

FRZ: -139°F

from OSHA Occupational Chemical DB

-139° F (NTP, 1992)

from CAMEO Chemicals

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13.1.5 Skin Symptoms

Dry skin. Redness.

► from ILO-ICSC

13.1.6 Eye Symptoms

Redness. Pain.

► from ILO-ICSC

13.1.7 Ingestion Symptoms

Burning sensation. Abdominal pain. Further see Inhalation.

► from ILO-ICSC

13.1.8 Target Organs

Eyes, skin, respiratory system, central nervous system, liver, kidneys

► from NIOSH-PocketGuide

Cardiovascular (Heart and Blood Vessels), Neurological (Nervous System)

► from CDC-ATSDR Toxic Substances Portal

13.1.9 Acute Toxicity Link

Chemical: TOLUENE

► from USGS Columbia Environmental Research Center

13.1.10 Acute Effects

The CNS is the primary target organ for toluene toxicity in both humans and animals for acute and chronic exposures. CNS dysfunction (which is often reversible) and narcosis have been frequently observed in humans acutely exposed to low or moderate levels of toluene by inhalation; symptoms include fatigue, sleepiness, headaches, and nausea. CNS depression and death have occurred at higher levels of exposure.

Cardiac arrhythmia has also been reported in humans acutely exposed to toluene.

Following the ingestion of toluene a person died from a severe depression of the CNS. Constriction and necrosis of myocardial fibers, swollen liver, congestion and hemorrhage of the lungs, and tubular kidney necrosis were also reported.

Save or download the
information on browser

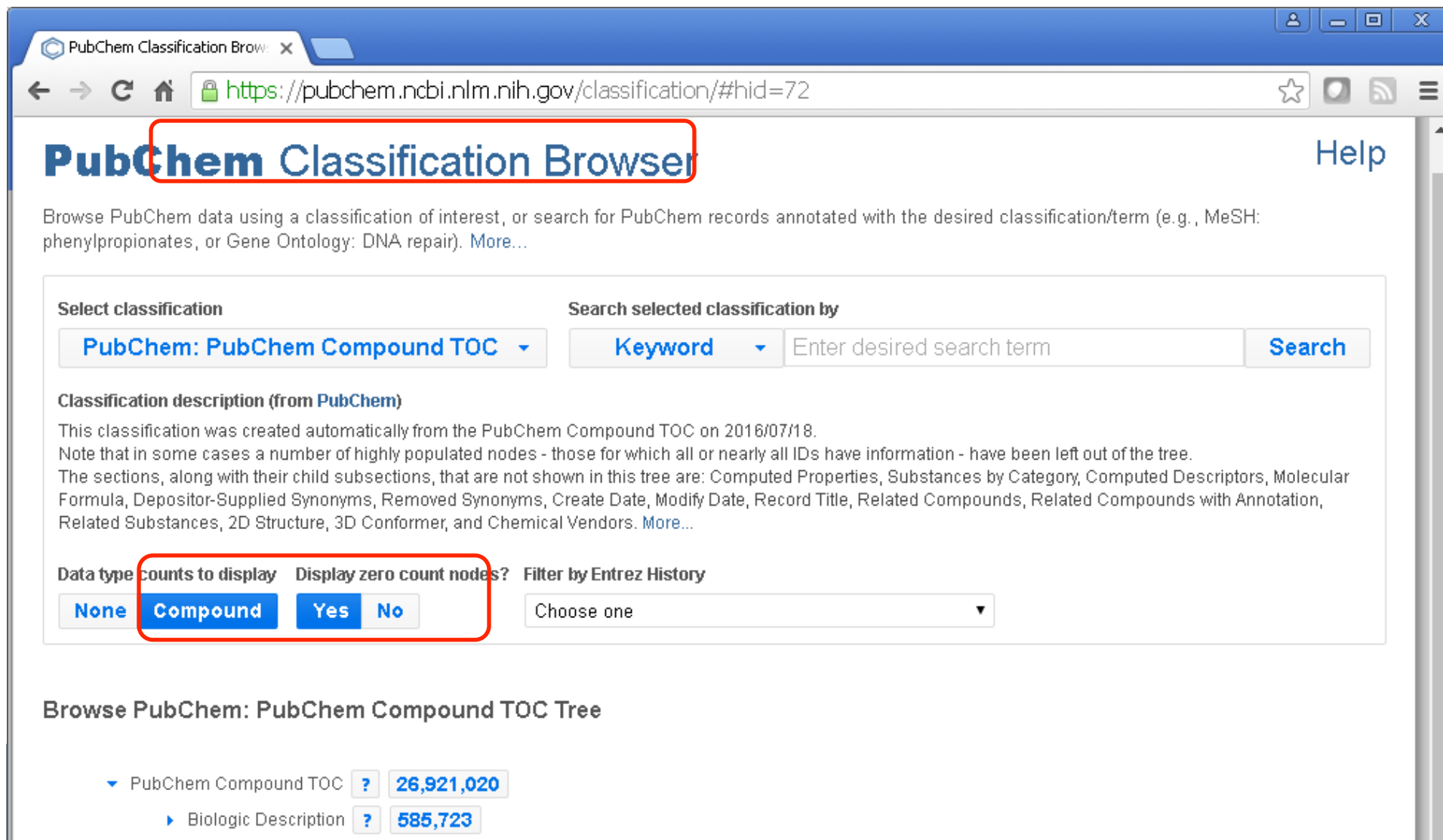
https://pubchem.ncbi.nlm.nih.gov/rest/pug_view/data/compound/1140/JSON/?response_type=display

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        "Section": [
          {
            "TOCHeading": "Record Title",
            "Description": "Text used as the title for this PubChem record",
            "Information": [
              {
                "ReferenceNumber": 35,
                "Name": "Record Title",
                "StringValue": "toluene"
              }
            ]
          },
          {
            "TOCHeading": "Record Description",
            "Description": "Textual summary about this PubChem record"
          }
        ]
      }
    ]
  }
}
```

Where to find the Information

- Get safety and hazard information for a given chemical
- Get all compounds that have safety and hazard annotations
- Retrieve safety and hazard information programmatically

Get all compounds that have safety and hazard annotations



PubChem Classification Browser

Help

Browse PubChem data using a classification of interest, or search for PubChem records annotated with the desired classification/term (e.g., MeSH: phenylpropionates, or Gene Ontology: DNA repair). [More...](#)

Select classification: PubChem: PubChem Compound TOC

Search selected classification by: Keyword

Enter desired search term

Search

Classification description (from PubChem)

This classification was created automatically from the PubChem Compound TOC on 2016/07/18. Note that in some cases a number of highly populated nodes - those for which all or nearly all IDs have information - have been left out of the tree. The sections, along with their child subsections, that are not shown in this tree are: Computed Properties, Substances by Category, Computed Descriptors, Molecular Formula, Depositor-Supplied Synonyms, Removed Synonyms, Create Date, Modify Date, Record Title, Related Compounds, Related Compounds with Annotation, Related Substances, 2D Structure, 3D Conformer, and Chemical Vendors. [More...](#)

Data type counts to display: None Compound Yes No

Display zero count nodes?: Yes No

Filter by Entrez History: Choose one

Browse PubChem: PubChem Compound TOC Tree

- PubChem Compound TOC ? 26,921,020
 - Biologic Description ? 585,723

121225388
121225360
121215529
119090965
119081209
119077305
119075735
119057962
119057958
119057957
119057832
119057828
119057809
119057737
119057735
119057734
119057364
119057361
119057340
119057336
118987278
118984465
118984459
118984398
118984389
118984355
118984354
118856763
118856642
118856472
....

Exported CIDs

PubChem Classification Browser: x

https://pubchem.ncbi.nlm.nih.gov/classification/#hid=72

Browse PubChem: PubChem Compound TOC Tree

- ▼ PubChem Compound TOC ? 26,921,020
 - ▶ Biologic Description ? 585,723
 - ▶ Biological Test Results ? 2,261,888
 - ▶ Biomolecular Interactions and Pathways ? 46,437
 - ▶ Chemical and Physical Properties ? 380,955
 - ▶ Classification ? 15,300,086
 - ▶ Drug and Medication Information ? 7,753
 - ▶ Food Additives and Ingredients ? 3,464
 - ▶ Identification ? 5,506
 - ▶ Information Sources ? 15,642,758
 - ▶ Literature ? 340,441
 - ▶ Names and Identifiers ? 226,489
 - ▶ Patents ? 17,995,278
 - ▶ Pharmacology and Biochemistry ? 20,752
 - ▶ Preparation and Reactions ?
 - ▶ Related Records ? 5,324,920
 - ▼ Safety and Hazards ? 11,487
 - ▶ Accidental Release Measures ? 8,022
 - ▶ Exposure Control and Personal Protection ? 6,828
 - ▶ Fire Fighting Measures ? 6,044
 - ▶ First Aid Measures ? 5,201
 - ▶ Handling and Storage ? 6,875
 - ▼ Hazards Identification ? 8,690
 - CLP Hazard Class and Category Codes ?
 - Explosion Hazard ? 905

Click the 5060 link will show the entrez compound page, then from the "Send to" button to save the 5060 CIDs as a text file.

Where to find the Information

- Get safety and hazard information for a given chemical
- Get all compounds that have safety and hazard annotations
- Retrieve safety and hazard information programmatically

Retrieve information programmatically using PubChem's PUG_View service

Data driven model: PubChem's pug_view service sends the json blob to the front end, the front end using script and css to render the page.

[https://pubchem.ncbi.nlm.nih.gov/rest/pug_view/data/
compound/1140/JSON](https://pubchem.ncbi.nlm.nih.gov/rest/pug_view/data/compound/1140/JSON)

[https://pubchem.ncbi.nlm.nih.gov/rest/pug_view/data/
compound/1140/XML](https://pubchem.ncbi.nlm.nih.gov/rest/pug_view/data/compound/1140/XML)

https://pubchem.ncbi.nlm.nih.gov/rest/pug_view/data/compound/1140/JSON/?response_type=dis

```
{
  "Record": {
    "RecordType": "CID",
    "RecordNumber": 1140,
    "Section": [
      {
        "TOCHeading": "2D Structure",
        "Description": "A two-dimensional representation of the compound.",
        "Information": [
          {
            "ReferenceNumber": 35,
            "Name": "2D Structure",
            "BoolValue": true
          }
        ]
      },
      {
        "TOCHeading": "3D Conformer",
        "Description": "A three-dimensional representation of the compound. The 3-D structure is not experimentally
determined, but computed by PubChem. More detailed information on this conformer model is described in the <a
href=\"http://www.springeropen.com/collections/PubChem3D\">PubChem3D thematic series </a> published in the Journal of
Cheminformatics. <a href=\"//pubchem.ncbi.nlm.nih.gov/docs/subcmpd_summary_page_help.html#3DConformer\">Read more...
</a>",
        "Information": [
          {
            "ReferenceNumber": 35,
            "Name": "3D Conformer",
            "Description": "toluene",
            "NumValue": 1140
          }
        ]
      },
      {
        "TOCHeading": "LCSS",
        "Description": "Whether this compound has an LCSS summary.",
        "Information": [
          {
            "ReferenceNumber": 35,
            "Name": "LCSS",
            "BoolValue": true
          }
        ]
      }
    ]
  }
}
```

Pug_view – Partial data retrieval

```
{
  "Record": {
    "RecordType": "CID",
    "RecordNumber": 1140,
    "Section": [
      {
        "TOCHeading": "Chemical and Physical Properties",
        "Description": "Chemical and physical properties such as melting point, molecular weight, etc.",
        "Section": [
          {
            "TOCHeading": "Experimental Properties",
            "Description": "Properties determined experimentally (See also Safety and Hazard Properties section for more information if available)",
            "Section": [
              {
                "TOCHeading": "Physical Description",
                "Description": "Physical description in general",
                "Information": [
                  {
                    "ReferenceNumber": 2,
                    "Name": "Physical Description",
                    "StringValue": "COLOURLESS LIQUID WITH CHARACTERISTIC ODOUR."
                  },
                  {
                    "ReferenceNumber": 3,
                    "Name": "Physical Description",
                    "StringValue": "Colorless liquid with a sweet, pungent, <a class='pubchem-internal-link CID-241\"
href='\"https://pubchem.ncbi.nlm.nih.gov/compound/benzene\">benzene</a>-like odor."
                  },
                  {
                    "ReferenceNumber": 4,
                    "Name": "Physical Description",
                    "StringValue": "Colorless liquid with a sweet, pungent, <a class='pubchem-internal-link CID-241\"
href='\"https://pubchem.ncbi.nlm.nih.gov/compound/benzene\">benzene</a>-like odor."
                  },
                  {
                    "ReferenceNumber": 13,
                    "Name": "Physical Description",
                    "StringValueList": [
                      "GasVapor, Liquid",
                      "Liquid",
                      "WetSolid"
                    ]
                  }
                ],
                "ReferenceNumber": 28,
                "Name": "Physical Description",
                "StringValue": "<a class='pubchem-internal-link CID-1140\" href='\"https://pubchem.ncbi.nlm.nih.gov/compound/Toluene\">Toluene</a> is a clear colorless
liquid with a characteristic aromatic odor. Flash point 40°F. Less dense than <a class='pubchem-internal-link CID-962\"
href='\"https://pubchem.ncbi.nlm.nih.gov/compound/water\">water</a> (7.2 lb / gal) and insoluble in <a class='pubchem-internal-link CID-962\"
href='\"https://pubchem.ncbi.nlm.nih.gov/compound/water\">water</a>. Hence floats on <a class='pubchem-internal-link CID-962\"
href='\"https://pubchem.ncbi.nlm.nih.gov/compound/water\">water</a>. Vapors heavier than air. May be toxic by inhalation, ingestion or skin contact. Used in aviation and
```

PubChem LCSS – A subset

The image displays three overlapping browser windows showing the PubChem LCSS (Laboratory Chemical Safety Summary) interface for Toluene (CID 1140).

Left Window: Shows the main title "Toluene" and the PubChem CID: 1140. It includes a chemical structure icon and a list of chemical names and molecular formula. The "Contents" section lists 13 items: 1 GHS Classification, 2 Identifiers, 3 Physical Properties, 4 Toxicity Data, 5 Exposure Limits, 6 Health and Symptoms, 7 First Aid, 8 Flammability and Explosivity, 9 Stability and Reactivity, 10 Storage and Handling, 11 Cleanup and Disposal, 12 Additional Considerations, and 13 Information Sources.

Middle Window: Shows the "Contents" section with a list of 13 items: 1 GHS Classification, 2 Identifiers, 3 Physical Properties, 4 Toxicity Data, 5 Exposure Limits, 6 Health and Symptoms, 7 First Aid, 8 Flammability and Explosivity, 9 Stability and Reactivity, 10 Storage and Handling, 11 Cleanup and Disposal, 12 Additional Considerations, and 13 Information Sources.

Right Window: Shows a sidebar with a "Help" icon and a "Link to this Record" button. It also includes a "Link to this Record" button and a "Link to this Record" button.

toluene | C6H5CH3 - PubChem

LCSS Laboratory Chemical Safety Summary for CID 1140

Contents

- 1 GHS Classification
- 2 Identifiers
 - 2.1 CAS
 - 2.2 InChI
 - 2.3 InChI Key
- 3 Physical Properties
 - 3.1 Physical Description
 - 3.2 Odor
 - 3.3 Boiling Point
 - 3.4 Melting Point
 - 3.5 Flash Point
 - 3.6 Solubility
 - 3.7 Density
 - 3.8 Vapor Density
 - 3.9 Vapor Pressure
 - 3.10 Auto-Ignition
 - 3.11 Decomposition
 - 3.12 Corrosivity
 - 3.13 Odor Threshold
- 4 Toxicity Data
 - 4.1 Non-Human Toxicity Values
- 5 Exposure Limits
 - 5.1 IDLH
 - 5.2 REL
 - 5.3 PEL
 - 5.4 PEL-TWA
 - 5.5 PEL-STEL
 - 5.6 REL-TWA
 - 5.7 REL-STEL
 - 5.8 Threshold Limit Values
 - 5.9 Occupational Exposure Limits
 - 5.10 Effects of Short Term Exposure
 - 5.11 Effects of Long Term Exposure
 - 5.12 Explosive Limits and Potential
 - 5.13 Allowable Tolerances
- 6 Health and Symptoms
 - 6.1 Symptoms
 - 6.2 Carcinogen
 - 6.3 Exposure Routes
- 6.3 Exposure Routes
- 6.4 Target Organs
- 6.5 Fire Hazard
- 6.6 Explosion Hazard
- 6.7 Hazards Summary
- 6.8 Fire Potential
- 6.9 Skin, Eye, and Respiratory
- 7 First Aid
 - 7.1 Inhalation First Aid
 - 7.2 Skin First Aid
 - 7.3 Eye First Aid
 - 7.4 Ingestion First Aid
- 8 Flammability and Explosivity
 - 8.1 Flammability
 - 8.2 LEL
 - 8.3 UEL
 - 8.4 NFPA Hazard Classification
 - 8.5 NFPA Fire Rating
 - 8.6 NFPA Health Rating
 - 8.7 Critical Temperature
 - 8.8 Critical Pressure
- 9 Stability and Reactivity
 - 9.1 Reactivities and Incompatibilities
- 10 Storage and Handling
 - 10.1 Safe Storage
 - 10.2 Storage Conditions
 - 10.3 Protective Equipment and Clothing
 - 10.4 Personal Protection
 - 10.5 Respirator Recommendations
 - 10.6 Nonfire Spill Response
- 11 Cleanup and Disposal
 - 11.1 Spillage Disposal
 - 11.2 Cleanup Methods
 - 11.3 Disposal Methods
- 12 Additional Considerations
 - 12.1 Toxic Combustion Products
- 13 Information Sources

1 GHS Classification

https://pubchem.ncbi.nlm.nih.gov/compound/toluene#datasheet=lc...



Toluene

[Cite this Record](#)

Vendors



Drug Information



Pharmacology



Literature



Patents



Bioactivities

**PubChem CID:** 1140**Chemical Names:** Toluene; Methylbenzene; Toluol; Methylbenzol; Phenylmethane; 108-88-3;[More...](#)**Molecular Formula:** C₆H₅CH₃ or C₇H₈**Molecular Weight:** 92.13842 g/mol**InChI Key:** YXFVABEGXRONW-UHFFFAOYSA-N**UNII:** 3FPU23BC52**Safety Summary:** [Laboratory Chemical Safety Summary \(LCSS\)](#)**Modify Date:** 2016-07-30**Create Date:** 2004-09-16

Toluene is a widely used industrial solvent.

[from MeSH](#)

Toluene is added to gasoline, used to produce [benzene](#), and used as a solvent. Exposure to toluene may occur from breathing ambient or indoor air affected by such sources. The central nervous system (CNS) is the primary target organ for toluene toxicity in both humans and animals for acute (short-term) and chronic (long-term) exposures. CNS dysfunction and narcosis have been frequently observed in humans acutely exposed to elevated airborne levels of toluene; symptoms include fatigue, sleepiness, headaches, and nausea. CNS depression has been reported to occur in chronic abusers exposed to high levels of toluene. Chronic inhalation exposure of humans to toluene also causes irritation of the upper respiratory tract and eyes, sore throat, dizziness, and headache. Human studies have reported developmental effects, such as CNS dysfunction, attention deficits, and minor craniofacial and limb anomalies, in the children of pregnant women exposed to high levels of toluene or mixed solvents by inhalation. EPA has concluded that there is inadequate information to assess the carcinogenic potential of toluene.

PubChem LCSS - URL

<https://pubchem.ncbi.nlm.nih.gov/compound/toluene#datasheet=lcss>

#datasheet=lcss



U.S. National Library of Medicine



Additional Safety Related Information

- GHS Classification

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

- Emergency Response Guidebook 2016

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

GHS Classification










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

GHS Classification

GHS, Globally Harmonized System of Classification and Labeling of Chemicals, was developed by the United Nations as a way to bring into agreement the chemical regulations and standards of different countries. GHS includes criteria for the classification of health, physical and environmental hazards, as well as specifying what information should be included on labels of hazardous chemicals as well as safety data sheets. Ref: [UNECE GHS \(Rev.6\) \(2015\)](#)

[Hazard Class Pictograms](#)
[GHS Hazard Statements](#)
[EU Hazard Statements](#)
[SWA Hazard Statements](#)
[Precautionary Statements](#)

Hazard Class Pictograms

 Exploding Bomb Explosives GHS01	 Flame Flammables GHS02	 Flame Over Circle Oxidizers GHS03
 Gas Cylinder Compressed Gases GHS04	 Corrosion Corrosives GHS05	 Skull and Crossbones Acute Toxicity GHS06
 Exclamation Mark Irritant GHS07	 Health Hazard GHS08	 Environment GHS09

GHS Hazard Statements

Code	Hazard Statements	Hazard Class	Category	Pictogram	Signal Word	Precautionary Statements P-Codes			
						Prevention	Response	Storage	Disposal

Emergency Response Guidebook 2016

The 2016 Emergency Response Guidebook, developed jointly by Transport Canada (TC), the U.S. Department of Transportation (DOT), the Secretariat of Communications and Transport of Mexico (SCT) and with the collaboration of CIQUIME (Centro de Información Química para Emergencias) of Argentina, provides first responders during the initial phase of a transportation incident involving dangerous goods and hazardous materials. This page provides a quick lookup table for related information.

References:

- [1] [The Emergency Response Guidebook website at PHMSA/DOT.](#)
- [2] The 2016 Emergency Response Guidebook in PDF: [English](#) and [Spanish](#).
- [3] The 2016 Emergency Response Guidebook [Data File Download \(spreadsheets\)](#).

UN Number	Guide Number	Material Name	TIH*	WR*	CB*
	112	Ammonium nitrate-fuel oil mixtures			
	158	Biological agents			
	112	Blasting agent, n.o.s.			
	112	Explosives, division 1.1, 1.2, 1.3 or 1.5			
	114	Explosives, division 1.4 or 1.6			
	153	Toxins			
1001	116	Acetylene, dissolved			
1002	122	Air, compressed			
1003	122	Air, refrigerated liquid (cryogenic liquid)			
1003	122	Air, refrigerated liquid (cryogenic liquid), non-pressurized			
1005	125	Ammonia, anhydrous	X		
1005	125	Anhydrous ammonia	X		

Summary

- PubChem provides chemical safety and hazard information that integrated from various open sources include NIOSH, ILO, HSDB, OSHA, NOAA Cameo Chemicals, ECHA, and more.
- PubChem created a subset chemical safety information page - LCSS.
- PubChem added GHS help page and DOT's EGR look up table.

Acknowledgements

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