

CINF80: 252nd ACS National Meeting, Philadelphia, PA, August 2016

# 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 screenshot shows a web browser window with multiple tabs. The active tab is titled "Deadly accident sounds alarm" and displays the Chemistry World website. The URL in the address bar is [www.rsc.org/chemistryworld/2016/01/tsinghua-university-postdoc-death-accident-chinese-lab-safety](http://www.rsc.org/chemistryworld/2016/01/tsinghua-university-postdoc-death-accident-chinese-lab-safety). The website header includes the "chemistryworld" logo, navigation links for SHOP, BLOG, NEWS, OPINIONS, FEATURES, REGULARS, JOBS, PODCASTS, and WEBINARS, and a search bar. A sidebar on the left contains a list of stories and social media sharing options. The main content area features a large banner for Agilent 6470 Triple Quadrupole LC/MS, followed by the article title "Deadly accident sounds alarm for safety in Chinese labs" by Hepeng Jia, dated 18 January 2016. The article text discusses a lab blast at Tsinghua University and the need for improved lab safety. A photo of a building is shown below the text. To the right of the article is an advertisement for Hiden Analytical's QGA Gas Analyser, listing features like high sensitivity and wide dynamic range. Below the advertisement is a "Related Content" section with a link to "California lab safety centre to investigate Hawaii University accident".

chemistryworld

SHOP FIND A JOB BLOG REGISTER

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RESEARCH BUSINESS NEWS AND ANALYSIS

ROCK SOLID LC/MS Agilent 6470 Triple Quadrupole LC/MS FIND OUT MORE

## Deadly accident sounds alarm for safety in Chinese labs

18 January 2016 Hepeng Jia

Like 699 Tweet G+ 2 Share 30

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

CLICK HERE TO FIND OUT MORE

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 screenshot shows the PubChem Project homepage in a web browser. The browser's address bar displays the URL <https://pubchem.ncbi.nlm.nih.gov>. The main content area features a table with the following data:

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

To the right of the table is a sidebar with social media icons (Facebook, Twitter, Google+, RSS, and a chat icon) and a list of tools: BioAssay Tools, Structure Search, 3D Conformer Tools, Structure Clustering, Classification, Upload, Download, and PubChem FTP. Below the table, there is a "more ..." link with an RSS icon. At the bottom of the page, there are links for "Write to Helpdesk", "Disclaimer", "Privacy Statement", "Accessibility", and "Data Citation Guidelines", along with the text "National Center for Biotechnology Information" and "NLM | NIH | HHS".

# 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
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- 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 Protection	Eye Prevention	TSCA Requirements
Chemical Dangers	REL	Ingestion Prevention	RCRA Requirements
Explosive Limits and Potential	PEL	Protective Equipment and Clothing	FIFRA Requirements
OSHA Standards	PEL-TWA	Stability and Reactivity	FDA Requirements
NIOSH Recommendations	PEL-STEL	Air and Water Reactions	Other Safety Information
Other Safety and Hazard Data	PEL-C	Reactive Group	Safety References
First Aid Measures	REL-TWA	Reactivity Alerts	Safety Notes
First Aid		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



# 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

# 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 for "toluene pubchem". The search bar contains the text "toluene pubchem" and is highlighted with a red box. The search results are displayed below the search bar, showing the top result for "toluene | C6H5CH3 - PubChem". The results include the PubChem URL, a brief description of toluene, and its chemical properties. Below the main result, there are several related compounds listed in a grid format, including Toluene-D8, Dibenzyl toluene, 4-Ethyltoluene, P-Toluenesulfonamide, Toluene-3,4-dithiol, and 2-Chlorotoluene. At the bottom of the page, there are logos for NIH and NCBI.

Toluene pubchem - Google S... x

https://www.google.com/#q=Toluene+pubchem

Google toluene pubchem

All Images Shopping News Videos More Search tools

About 56,300 results (0.29 seconds)

**toluene | C6H5CH3 - PubChem**  
<https://pubchem.ncbi.nlm.nih.gov/compound/toluene> PubChem  
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 ...  
PubChem CID: 1140 Molecular Weight: 92.13842 g/mol  
Chemical Names: Toluene; Methylbenz... Molecular Formula: C<sub>6</sub>H<sub>5</sub>CH<sub>3</sub> or C<sub>7</sub>H<sub>8</sub>

**TOLUENE-D8**  
TOLUENE-D8 | C7H8 | CID 74861 - structure, chemical names ...

**Dibenzyl toluene**  
Dibenzyl toluene | C21H20 | CID 3034397 - structure, chemical ...

**4-Ethyltoluene**  
4-Ethyltoluene | C9H12 | CID 12160 - structure, chemical ...

**P-TOLUENESULFONAMIDE**  
P-TOLUENESULFONAMIDE | C7H9NO2S | CID 6269 ...

**TOLUENE-3,4-DITHIOL**  
TOLUENE-3,4-DITHIOL | C7H8S2 | CID 10334 - structure ...

**2-Chlorotoluene**  
2-Chlorotoluene | C1C6H4CH3 or CH3C6H4Cl or C7H7Cl | CID ...

[More results from nih.gov »](#)

**hydride toluene | C7H9- - PubChem**  
<https://pubchem.ncbi.nlm.nih.gov/compound/86595848> PubChem  
hydride toluene | C7H9- | CID 86595848 - structure, chemical names, physical and chemical properties, classification, patents, literature, biological activities, ...

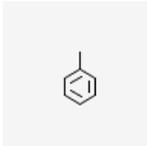
**benzoyl peroxide toluene | C21H18O4 - PubChem**

NIH NCBI

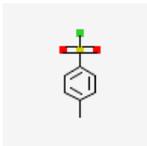
# Case study: toluene: from PubChem/Entrez

The screenshot displays the PubChem Compound search results for 'toluene'. The browser address bar shows the URL: <https://www.ncbi.nlm.nih.gov/pccompound/?term=toluene>. The search bar contains 'toluene' and the search button is labeled 'Search'. The page shows 10493 items, with the first three results listed below.

**Search results**  
Items: 1 to 20 of 10493

1.  [toluene; methylbenzene; toluol ...](#)  
MW: 92.138420 g/mol MF: C<sub>7</sub>H<sub>8</sub>  
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](#)

2.  [P-TOLUENESULFONIC ACID; 4-Methylbenzenesulfonic acid; 104-15-4 ...](#)  
MW: 172.201620 g/mol MF: C<sub>7</sub>H<sub>8</sub>O<sub>3</sub>S  
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](#)

3.  [Tosyl chloride; P-TOLUENESULFONYL CHLORIDE; 98-59-9 ...](#)  
MW: 190.647280 g/mol MF: C<sub>7</sub>H<sub>7</sub>ClO<sub>2</sub>S  
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](#)

4.  [2,4-Toluene diisocyanate; Toluene-2,4-diisocyanate; 2,4-Diisocyanatotoluene ...](#)  
MW: 174.155410 g/mol MF: C<sub>7</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>

**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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- 12 Safety and Hazards
- 13 Toxicity
- 14 Literature
- 15 Patents
- 16 Biomolecular Interactions and Pathways
- 17 Biological Test Results
- 18 Classification
- 19 Information Sources

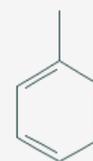
## 1 2D Structure



Search

Download

Get Image



Magnify

from PubChem

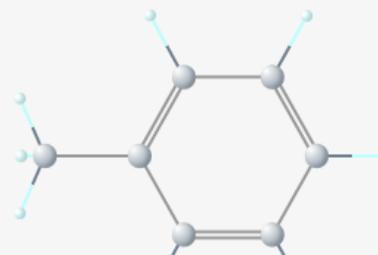
## 2 3D Conformer



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

### Contents

- 1 2D Structure
- 2 3D Conformer
- 3 Names and Identifiers
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    - 3.1.1 IUPAC Name
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    - 3.1.3 InChI Key
    - 3.1.4 Canonical SMILES
  - 3.2 Molecular Formula
  - 3.3 Other Identifiers
  - 3.4 Synonyms
    - 3.4.1 MeSH Synonyms
    - 3.4.2 Depositor-Supplied Synonyms
  - 4 Chemical and Physical Properties
    - 4.1 Computed Properties
    - 4.2 Experimental Properties
      - 4.2.1 Physical Description
      - 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

Download Print Share Help

### Contents

- 4 Chemical and Physical Properties
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    - 4.2.6 Flash Point
    - 4.2.7 Solubility
    - 4.2.8 Density
    - 4.2.9 Vapor Density
    - 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

toluene | C6H5CH3 - PubCh... x

← → ↻ 🏠 <https://pubchem.ncbi.nlm.nih.gov/compound/toluene#section=Skin-Symptoms> ☆ 📺 📄 ☰

🏠 Compound Summary for CID 1140

⬇️ Download 🖨️ Print 🔄 Share ? Help ⬆️

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    - 13.1.4 Inhalation Symptoms
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    - 13.1.19 Non-Human Toxicity Values

#### 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

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#### 13.1.9 Acute Toxicity Link

Chemical: [TOLUENE](#)

▶ from USGS Columbia Environmental Research Center

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#### 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

{
  "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": "LCSS",
            "BoolValue": true
          }
        ]
      },
      {
        "TOCHeading": "Names and Identifiers",
        "Description": "Information describing the identity of this PubChem Compound record, including record identifiers, synonyms (i.e., chemical names), descriptors, etc. <a href='\"//pubchem.ncbi.nlm.nih.gov/docs/subcmpd_summary_page_help.html#Identification\"'>Read more...</a>",
        "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"
      }
    ]
  }
}
```

https://pubchem.ncbi.nlm.nih.gov/rest/pug\_view/data/compound/1140/JSON/?response\_type=display

# 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: Compound

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

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

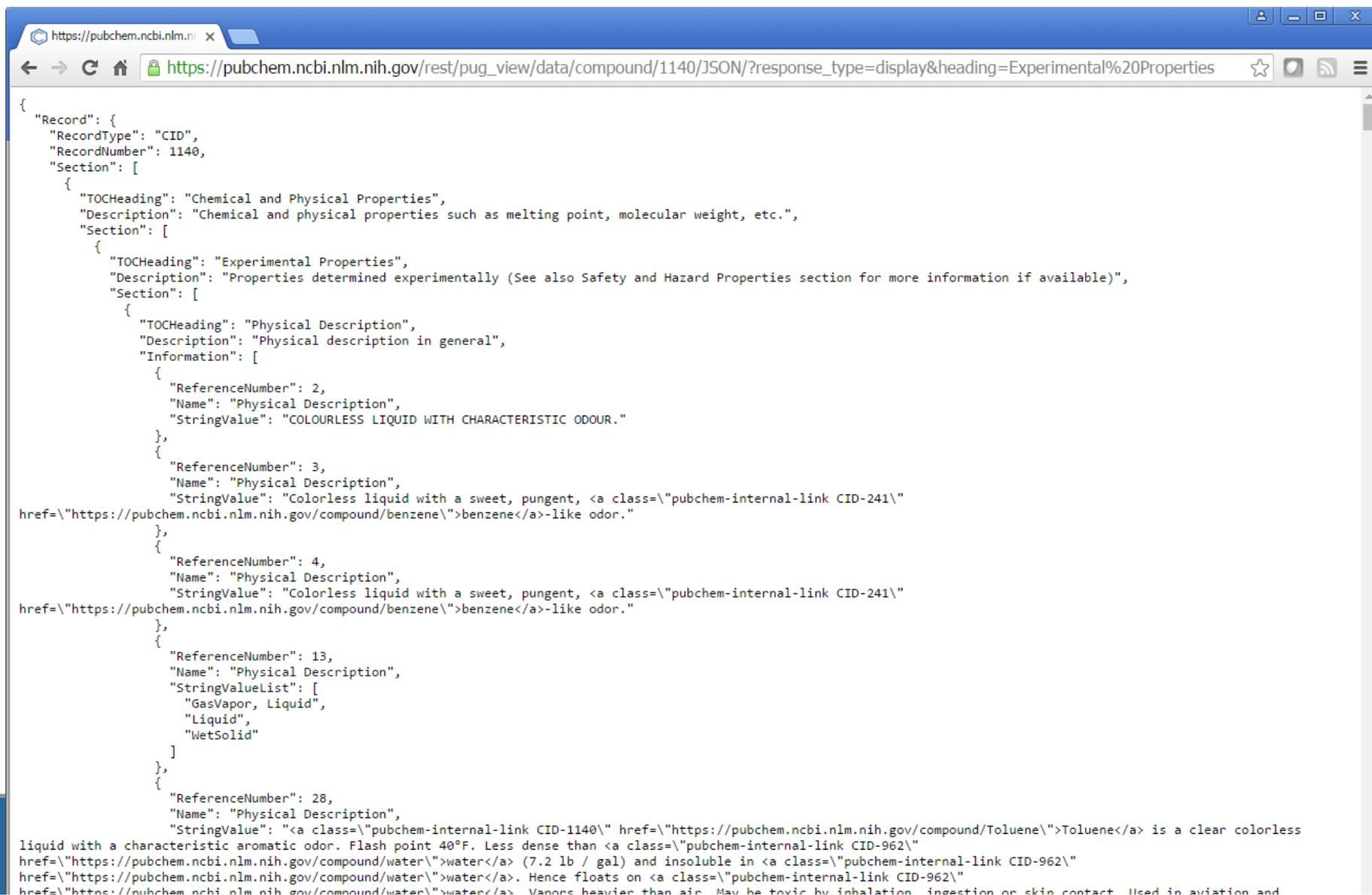
**Data driven model:** PubChem's pug\_view service sends the json blob to the front end, the front end using script and css to render the page.

[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). The leftmost window shows the main page with the title "Toluene" and a list of 13 content categories. The middle window shows the "Contents" section expanded, listing the same 13 categories. The rightmost window shows a detailed view of the "Toxicity Data" section, including hazard categories like "Category 1" and "Category 2B".

**Contents**

- 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
- 13 Information Sources

**Toxicity Data**

Category 1]

- Category 1]

Category 2B]

Category 1A,

exposure -

anger Specific

d - Category 2]

environment,

od.

on sources. - No

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:** C<sub>6</sub>H<sub>5</sub>CH<sub>3</sub> or C<sub>7</sub>H<sub>8</sub>**Molecular Weight:** 92.13842 g/mol**InChI Key:** YXFVVABEGXRONW-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

# 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

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*
	<a href="#">112</a>	Ammonium nitrate-fuel oil mixtures			
	<a href="#">158</a>	Biological agents			
	<a href="#">112</a>	Blasting agent, n.o.s.			
	<a href="#">112</a>	Explosives, division 1.1, 1.2, 1.3 or 1.5			
	<a href="#">114</a>	Explosives, division 1.4 or 1.6			
	<a href="#">153</a>	Toxins			
<a href="#">1001</a>	<a href="#">116</a>	Acetylene, dissolved			
<a href="#">1002</a>	<a href="#">122</a>	Air, compressed			
<a href="#">1003</a>	<a href="#">122</a>	Air, refrigerated liquid (cryogenic liquid)			
<a href="#">1003</a>	<a href="#">122</a>	Air, refrigerated liquid (cryogenic liquid), non-pressurized			
<a href="#">1005</a>	<a href="#">125</a>	Ammonia, anhydrous	X		
<a href="#">1005</a>	<a href="#">125</a>	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

PubChem Crew

Renata Geer

Jane He

Gang Fu

Sunghwan Kim

Bo Yu

Ben Shoemaker

Siqian He

Jiyao Wang

Jie Chen

Yanli Wang

Tiejun Cheng



U.S. National Library of Medicine

