Chemical Safety and Hazard Information in PubChem

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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.
Lab Accidents

Deadly accident sounds alarm for safety in Chinese labs

18 January 2016

Hepeng Jia

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 northwestern Chinese city of Yinchuan.

A female graduate student was killed when a flash fire started from a lab solvent in Kunming, a city in Yunnan Province, on 24 December. A female lab worker and a male research assistant were sent a hospital, with the latter remaining in critical condition. The investigation into the accident is ongoing.

Two high-school students were wounded with burns when an explosion occurred at a lab of a school in Nanchang City, Jiangxi Province. The incident happened on 15 December.

The accident has caused huge concern in the lab community. "Safeguarding the lives of students in the lab is the government's top priority," said a senior of the Education Ministry, "and we are stepping up our efforts to make sure our students can work in a secure environment in the lab."
Chemical Safety Information
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 or origin of 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
- Isobutylene
- 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 od 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/
• ![QR Code](image-url)
### PubChem Homepage

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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
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- 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
Hazards Identification
GHS Classification
CLP Hazard Class and Category Codes
Health Hazard
Fire Hazard
Explosion Hazard
Hazards Summary
Fire Potential
Skin, Eye, and Respiratory Irritations
Safety and Hazard Properties
LEL
UEL
Flammability
Critical Temperature
Critical Pressure
Danger of Explosion
NFPA Hazard Classification
NFPA Fire Rating
NFPA Reactivity Rating
NFPA Health Rating
NFPA Other
Physical Dangers
Chemical Dangers
Explosive Limits and Potential
OSHA Standards
NIOSH Recommendations
Other Safety and Hazard Data
First Aid Measures
First Aid
Fire First Aid
Explosion First Aid
Exposure First Aid
Inhalation First Aid
Skin First Aid
Eye First Aid
Ingestion First Aid
Fire Fighting Measures
Fire Fighting
Explosion Fire Fighting
Other Fire Fighting Hazards
Accidental Release Measures
TIH Gas
Isolation and Evacuation
Spillage Disposal
Cleanup Methods
Disposal Methods
Other Preventative Measures
Handling and Storage
Nonfire Spill Response
Safe Storage
Storage Conditions
Exposure Control and Personal Protection
REL
REL-C
REL-STEEL
IDLH
Conversion
Threshold Limit Values
Other Occupational Permissible Levels Sources and Potential Exposure
Assessing Personal Exposure
Occupational Exposure Limits
Inhalation Risk
Effects of Short Term Exposure
Effects of Long Term Exposure
Radiation Limits and Potential
Acceptable Daily Intakes
Allowable Tolerances
Personal Protection
Respirator Recommendations
Fire Prevention
Explosion Prevention
Exposure Prevention
Inhalation Prevention
Skin Prevention
Eye Prevention
Ingestion Prevention
Protective Equipment and Clothing
Stability and Reactivity
Air and Water Reactions
Reactive Group
Reactivity Alerts
Reactivity Profile

Reactivities and Incompatibilities
Transport Information
DOT Emergency Guidelines
Shipment Methods and Regulations
DOT ID and Guide
DOT Label
Packaging and Labelling
EC Classification
UN Classification
Emergency Response
Regulatory Information
DOT Emergency Response Guide
Isolation Name
Isolation Distance
Atmospheric Standards
Soil Standards
Federal Drinking Water Standards
Federal Drinking Water Guidelines
State Drinking Water Standards
State Drinking Water Guidelines
Clean Water Act Requirements
CERCLA Reportable Quantities
TSCA Requirements
RCRA Requirements
FIFRA Requirements
FDA Requirements
Other Safety Information
Safety References
Safety Notes
Toxic Combustion Products
Other Hazardous Reactions

Other Safety Data

Safety References
Safety Notes
Toxic Combustion Products
Other Hazardous Reactions
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

- EPA (United States Environmental Protection Agency)
- ILO (International Labour Organization)
- Safe Work Australia
- CDC
- Europa.eu
- ATSDR
- NIOSH
- United States Department of Labor
- TOXNET
- ECHA (European Chemicals Agency)
- PHMSA (Pipeline and Hazardous Materials Safety Administration)
- NJ Health
- OSHA
- NITE (National Institute of Technology and Evaluation)
- NIH (U.S. National Library of Medicine)
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
Case study: toluene: from PubChem/Entrez
Direct URL


Compound Summary for CID 1140

1 2D Structure

3 3D Conformer

Contents

1 2D Structure
2 3D Conformer
3 Names and Identifiers
4 Chemical and Physical Properties
5 Related Records
6 Chemical Vendors
7 Drug and Medication Information
8 Food Additives and Ingredients
9 Pharmacology and Biochemistry
10 Use and Manufacturing
11 Identification
12 Safety and Hazards
13 Toxicity
14 Literature
15 Patents
16 Biomolecular Interactions and Pathways
17 Biological Test Results
18 Classification
19 Information Sources

Magnify

From PubChem
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**

203-525-9

- from ECHA

3.3.3 **ICSC Number**

0078

- from ILO-ICSC

3.3.4 **RTECS Number**

X55250000

- from ILO-ICSC, NIOSH-PocketGuide

3.3.5 **UN Number**

1294

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

1294

- from Emergency Response Guidebook

3.3.6 **UNII**

3FPZ23BG52

- from FDA/SPL Indexing Data
4.2.3 Odor

Sweet, pungent, benzene-like odor.


4.2.4 Boiling Point

110.6 °C


111 °C

from NIOSH-PocketGuide, OSHA Occupational Chemical DB

232 °F

from ILO-ICSC

231.1 °F at 760.0 mm Hg (NTP, 1992)

from GAMEO Chemicals

4.2.5 Melting Point

-94.9 °C


-96 °C

from NIOSH-PocketGuide

-139 °F

from ILO-ICSC

FRZ: -139 °F

from OSHA Occupational Chemical DB

-139 °F (NTP, 1992)

from GAMEO Chemicals
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-ATSOR 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
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
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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.


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        "Description": "toluene",
        "NumValue": 1140
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    ]
  },
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  }
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To retrieve data for a specific heading, e.g., Experimental Properties, use:


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        "Description": "Chemical and physical properties such as melting point, molecular weight, etc."
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      {
        "TOCHeading": "Experimental Properties",
        "Description": "Properties determined experimentally (See also Safety and Hazard Properties section for more information if available)"
      },
      {
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        "Description": "Physical description in general"
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      }
    ]
  }
}
```
PubChem LCSS – A subset
Toluene is a widely used industrial solvent. 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

Additional Safety Related Information

• GHS Classification

• Emergency Response Guidebook 2016
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

<table>
<thead>
<tr>
<th>Exploding Bomb</th>
<th>Flame</th>
<th>Flame Over Circle</th>
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<tbody>
<tr>
<td>Explosives GHS01</td>
<td>Flammable GHS02</td>
<td>Oxidizers GHS03</td>
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<tr>
<td>Gas Cylinder</td>
<td>Corrosion</td>
<td>Skull and Crossbones</td>
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<td>Compressed Gases GHS04</td>
<td>Corrosives GHS05</td>
<td>Acute Toxicity GHS06</td>
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<td>Exclamation Mark</td>
<td>Health Hazard</td>
<td>Environment</td>
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<tr>
<td>Irritant GHS07</td>
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GHS Hazard Statements

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<tr>
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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:


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<td></td>
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<td>Air, refrigerated liquid (cryogenic liquid)</td>
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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.
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