

PubChem's Laboratory Chemical Safety Summary (LCSS)

Sunghwan Kim¹ (kimsungh@ncbi.nlm.nih.gov), Jian Zhang¹, Asta Gindulyte¹, Paul Thiessen¹, Leah McEwen², Ralph Stuart³, Evan E. Bolton¹, Stephen H. Bryant¹

¹ National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health

² Clark Physical Science Library, Cornell University.

³ Office of Environmental Health & Safety, Keene State College,

□ Acknowledgements

▪ The PubChem Team

Stephen Bryant

Evan E. Bolton

Lewis Geer

Yanli Wang

Asta Gindulyte

Lianyi Han

Bo Yu

Paul Thiessen

Jian Zhang

Jiyao Wang

Renata Geer

Ben Shoemaker

Jane He

Jie Chen

Tiejun Cheng

Gang Fu

Leonid Zaslavsky

Takako Takeda

Ming Hao

Amrita Roy Choudhury

▪ PubChem depositors, users, and collaborators

▪ Funded by the National Library of Medicine

▪ Leah McEwen (Cornell) & Ralph Stuart (Keene State)

□ PubChem Presentations at ACS San Diego

- 10 presentations has been given already.
- 3 more presentations will be given tomorrow.
- See the PubChem Blog for a list of PubChem presentations (<https://pubchemblog.ncbi.nlm.nih.gov>).

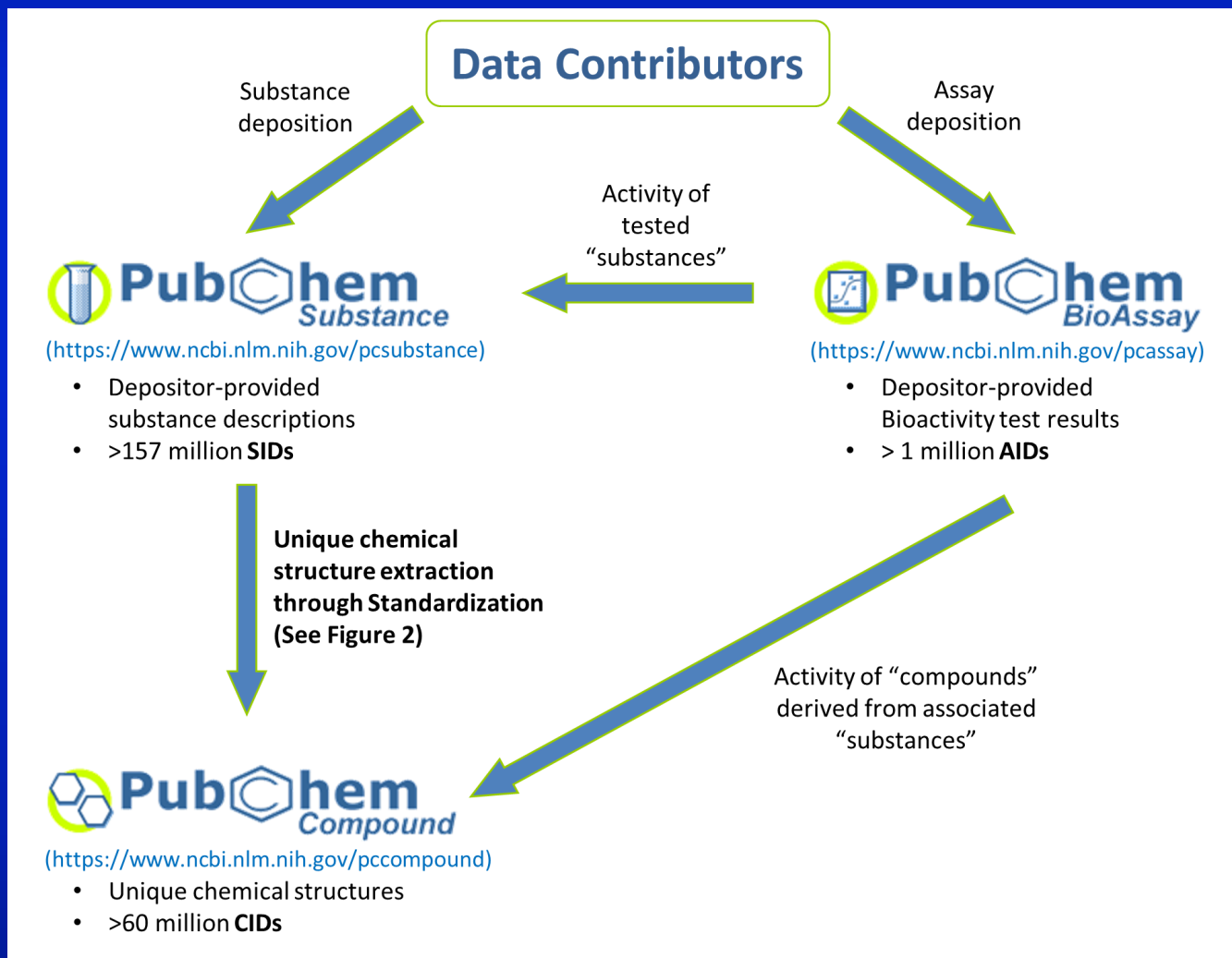
PubChem

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

□ PubChem (<https://pubchem.ncbi.nlm.nih.gov>)

- A “public” repository of information on small molecules and their biological activities, developed and maintained by the U.S. National Institutes of Health (NIH).
- Launched in 2004 as a part of the Molecular Libraries Roadmap initiatives.
- A key resource of chemical information for researchers in the area of cheminformatics, chemical biology, medicinal chemistry, and many others.

□ PubChem (<https://pubchem.ncbi.nlm.nih.gov>)

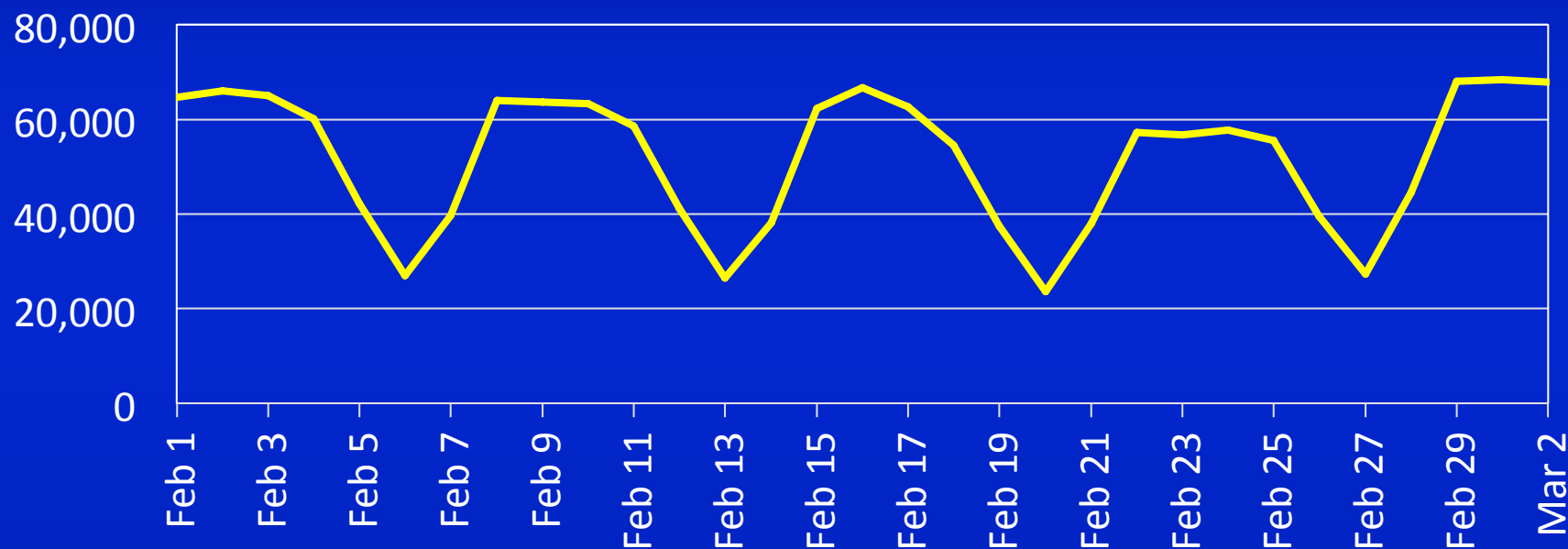


□ PubChem (<http://pubchem.ncbi.nlm.nih.gov>)

- PubChem contains:
 - >218 million substance descriptions,
 - >88 million unique chemical structures,
 - >229 million biological test results
 - >1 million biological assays, covering ~10,000 unique protein sequence targets.

(Arguably) the largest corpus of publicly available chemical information from more than 400 data contributors.

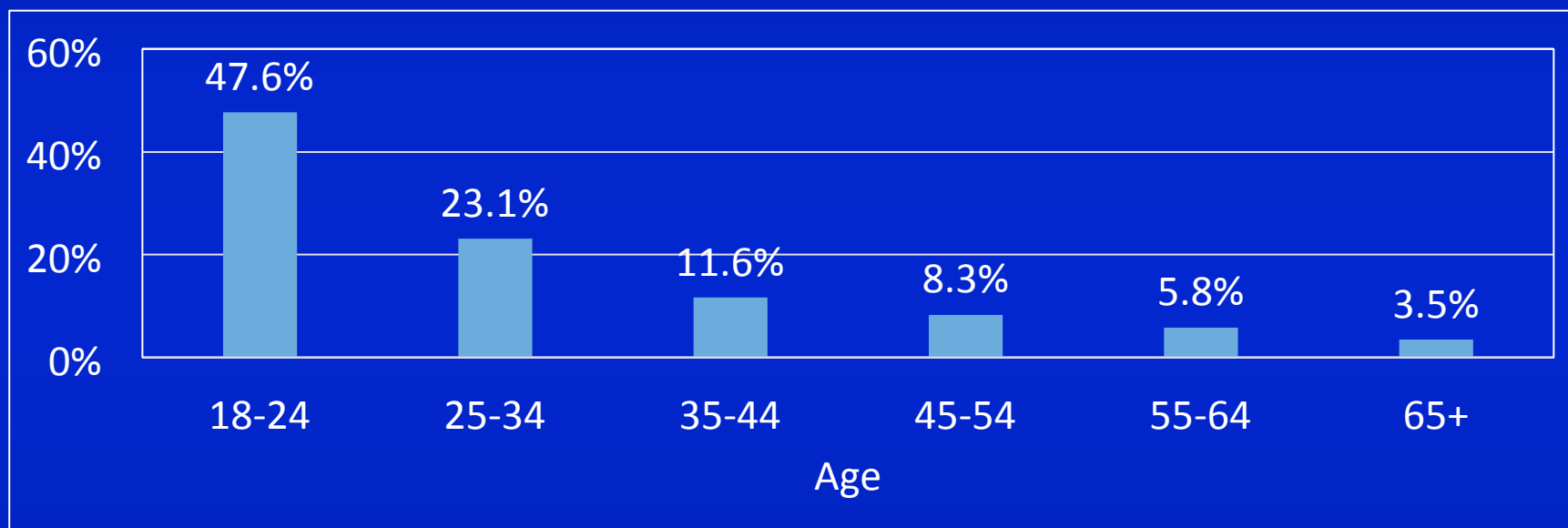
Number of PubChem Users



- For the 30-day period (between Feb. 1 – Mar. 2, 2016)
 - Average daily users: **51,871**
 - Unique users for the past 30 days: **1,201,813**

Demographics of PubChem Users

among 467,671 users (45.6 % of 1,026,283 Users)



- ~50% of PubChem users are at **age 18-24**
- **They are likely to be students**

PubChem
Laboratory Chemical Safety Summary
(LCSS)

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

□ PubChem LCSS

- A concise view of health and safety data for a given compound.

- Flammability
- Toxicity
- Exposure limits
- Exposure symptoms
- First aid
- Handling
- Spill clean up
- Many others

NIH > NLM > National Center for Biotechnology Information

PubChem OPEN CHEMISTRY DATABASE

Search Compounds

LCSS Laboratory Chemical Safety Summary for CID 8028

Download Print Share Help

PUBCHEM > COMPOUND > TETRAHYDROFURAN > LCSS

Read about the LCSS project

TETRAHYDROFURAN

Cite this Record

PubChem CID: 8028

Chemical Names: TETRAHYDROFURAN; Oxolane; Furanidine; Butylene oxide; 109-99-9; Furan, tetrahydro-

Molecular Formula: C₄H₈O

Molecular Weight: 72.10572 g/mol

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

1 GHS Classification

Signal: Dgr
H225 - Highly flammable liquid and vapour
H351 - Suspected of causing cancer
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation

from REGULATION (EC) No 1272/2008

2 Identifiers

2.1 CAS

109-99-9

from EPA Chemical Data Report, ILO-ICSC, NIOSH-PocketGuide, OSHA Occupati...

2.2 InChI

InChI=1S/C4H8O/c1-2-4-5-3-1/h1-4H2

from PubChem

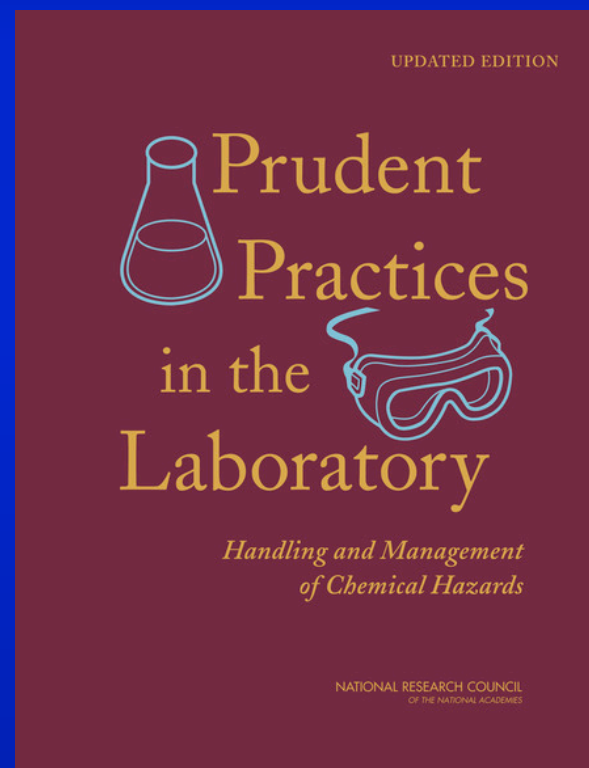
2.3 InChI Key

WYURNTSHIVDZCO-UHFFFAOYSA-N

from PubChem

□ PubChem LCSS

- Based on the format described by the National Research Council in “Prudent Practices in the Laboratory: Handling and Management of Chemical Hazards” (2011)



Free PDF available from

<http://www.nap.edu/catalog/12654/prudent-practices-in-the-laboratory-handling-and-management-of-chemical>.

□ PubChem LCSS

- Supports chemical risk assessment in laboratories
- Provides information relevant to use of chemicals as described in the OSHA lab standard[†].
→ Supplements the material safety data sheet (MSDS).

[†] *Toxic and Hazardous Substances: National Research Council Recommendations Concerning Chemical Hygiene in Laboratories (Non-Mandatory)*. 29 CFR §1910.1450 Appendix A. Occupational Safety and Health Administration (OSHA), Washington, DC, 2012.
https://www.osha.gov/pls/oshaweb/owadisp.show_document?p_table=STANDARDS&p_id=10107 (accessed Mar. 10, 2016).

□ PubChem LCSS Coverage

- Globally Harmonized System of Classification and Labeling of Chemicals (GHS)

(http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html)

- International standard for technical criteria for **classifying chemicals** according to their **health, physical, and environmental hazards**.



□ PubChem LCSS Coverage

- Globally Harmonized System of Classification and Labeling of Chemicals (GHS)

(http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html)


- Hazard communication requirements for product labels and safety data sheets.

Turpentine CAS No.: 8008-20-6

DANGER

Hazard Statements
Flammable liquid and vapor. Harmful if swallowed. May be fatal if swallowed and enters airways. Harmful in contact with skin. Causes skin irritation. May cause an allergic skin reaction. Causes serious eye irritation. Harmful if inhaled. Toxic to aquatic life with long lasting effects.

Precautionary Statements
Keep out of reach of children. Avoid release to the environment. Wear protective gloves/ protective clothing/ eye protection/ face protection.
If skin irritation occurs: Get medical advice/ attention.



Supplier Identification

CONSULT SDS FOR ADDITIONAL INFORMATION ON HAZARDS

□ PubChem LCSS Coverage

- Globally Harmonized System of Classification and Labeling of Chemicals (GHS)
(http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html)
- Global basis for harmonization of rules and regulations on hazardous chemicals
 - Improves regulatory efficiency
 - Facilitates international trades

□ PubChem LCSS Coverage

- PubChem LCSS is available for 5,130 compounds with GHS classification information

GHS classification source	# Compounds
EU REGULATION (EC) No 1272/2008 (a EU Regulation for classification, labelling and packaging of substances and mixtures)	3,263
International Chemical Safety Cards (ICSC) at International Labor Organization (ILO)	532
Chemical Management Center (CMC) at Japan National Institute of Technology and Evaluation (NITE)	2,723
Hazardous Substance Information System (HSIS) at Safe Work Australia	3,191
Total Unique Compounds	5,130

PubChem LCSS Data Contents

- GHS Classification
- Synonyms
- Identifiers
- Physical Properties
- Toxicity Data
- Exposure Limits
- Health and Symptoms
- First Aid
- Flammability & Explosivity
- **Stability and Reactivity**
- Storage and Handling
- Cleanup and Disposal
- Additional Considerations

Data contents in PubChem Laboratory Chemical Safety Summary (LCSS)

- As of October 30, 2015
- Abbreviations in brackets indicate data sources.

GHS Classification [CLP, ICSC]

Synonyms [PC]

Identifiers

PubChem CID [PC]
CAS [DRGBNK, EPA-CDR, ICSC, NIOSH, OSHA]
InChI [PC]
InChI Key [PC]

Physical Properties

Physical Description [CAMEO, EPA-CDR, ICSC, NIOSH, OSHA]
Odor [HSDB]
Boiling Point [CAMEO, DRGBNK, HSDB, ICSC, NIOSH, OSHA]
Melting Point [CAMEO, DRGBNK, HSDB, ICSC, NIOSH, OSHA]
Flash Point [HSDB, ICSC, NIOSH, OSHA]
Solubility [CAMEO, DRGBNK, HSDB, ICSC, NCI, NIOSH]
Density [CAMEO, HSDB, ICSC, NIOSH, OSHA]
Vapor Density [CAMEO, HSDB, ICSC, OSHA]
Vapor Pressure [CAMEO, HSDB, ICSC, NIOSH, OSHA]
Auto-Ignition [HSDB, ICSC]
Decomposition [HSDB, ICSC]
Corrosivity [HSDB]
Odor Threshold [HSDB]

Toxicity Data

Toxicity Summary [DRGBNK, HSDB]
Human Toxicity Values [HSDB]
Non-Human Toxicity Values [HSDB]

Exposure Limits

Immediately Dangerous to Life or Health Concentration [NIOSH, OSHA]
Recommended Exposure Limit (REL) [NIOSH, OSHA]
Permissible Exposure Limit (PEL) [NIOSH, OSHA]
REL-Time-Weighted Average Concentration (REL-TWAC) [OSHA]
REL-Short-Term Exposure Limit (REL-STEL) [OSHA]
REL-Ceiling (REL-C) [OSHA]
PEL-Time-Weighted Average Concentration (PEL-TWAC) [OSHA]
PEL-Short-Term Exposure Limit (PEL-STEL) [OSHA]
PEL-Ceiling (PEL-C) [OSHA]
Threshold Limit Values [HSDB]
Occupational Exposure Limits [ICSC]
Effects of Short Term Exposure [ICSC]
Effects of Long Term Exposure [ICSC]
Explosive Limits and Potential [HSDB, ICSC]
Radiation Limits and Potential [HSDB]
Acceptable Daily Intakes [HSDB]
Allowable Tolerances [HSDB]

Health and Symptoms

Symptoms [NIOSH]
Carcinogen [ATSDR, HSDB, OSHA]
Exposure Routes [ICSC, NIOSH]
Target Organs [ATSDR, NIOSH]
Cancer Sites [NIOSH]
Fire Hazard [ICSC]
Explosion Hazard [ICSC]
Exposure Hazard [ICSC]
Skin Hazard [ICSC]
Inhalation Hazard [ICSC]
Eye Hazard [ICSC]
Ingestion Hazard [ICSC]
Hazards Summary [ATSDR, EPA-AT, HSDB]
Fire Potential [HSDB]
Skin, Eye, and Respiratory Irritations [HSDB]

First Aid

Fire First Aid [ICSC]
Explosion First Aid [ICSC]
Exposure First Aid [ICSC]
Inhalation First Aid [ICSC]
Skin First Aid [ICSC]
Eye First Aid [ICSC]
Ingestion First Aid [ICSC]

Flammability and Explosivity

Flammability [HSDB, NIOSH]
Lower Explosive Limit (LEL) [NIOSH, OSHA]
Upper Explosive Limit (UEL) [NIOSH, OSHA]
NFPA Hazard Classification [HSDB]
NFPA Fire Rating [CAMEO, OSHA]
NFPA Reactivity Rating [CAMEO, OSHA]
NFPA Health Rating [CAMEO, OSHA]
NFPA Other [CAMEO, OSHA]
Critical Temperature [HSDB]
Critical Pressure [HSDB]

Stability and Reactivity

Reactivities and Incompatibilities [HSDB, NIOSH, OSHA]

Storage and Handling

Safe Storage [ICSC]
Storage Conditions [HSDB]
Protective Equipment and Clothing [HSDB]
Personal Protection [NIOSH]
Respirator Recommendations [NIOSH]
Nonfire Spill Response [OSHA]

Cleanup and Disposal

Spillage Disposal [ICSC]
Cleanup Methods [HSDB]
Disposal Methods [HSDB]

Additional Considerations

Toxic Combustion Products [HSDB]
Other Hazardous Reactions [HSDB]

[http://confchem.ccce.divched.org/sites/
confchem.ccce.divched.org/files/
2015FallCCCENLP3fig5.pdf](http://confchem.ccce.divched.org/sites/confchem.ccce.divched.org/files/2015FallCCCENLP3fig5.pdf)

PubChem LCSS Data Sources

- CDC ATSDR Toxic Substance Portal
- NOAA CAMEO Chemicals
- Regulation (EC) No 12 1272/2008
- DrugBank
- EPA Air Toxics
- EPA Chemical Data Report
- HSDB
- ILO ICSC
- NCI Investigational Drugs
- NIOSH Pocket Guide
- OSHA Occupational Chemical DB
- PubChem

Data contents in PubChem Laboratory Chemical Safety Summary (LCSS)

- As of October 30, 2015
- Abbreviations in brackets indicate data sources.

GHS Classification [CLP, ICSC]

Synonyms [PC]

Identifiers

- PubChem CID [PC]
- CAS [DRGBNK, EPA-CDR, ICSC, NIOSH, OSHA]
- InChI [PC]
- InChI Key [PC]

Physical Properties

- Physical Description [CAMEO, EPA-CDR, ICSC, NIOSH, OSHA]
- Odor [HSDB]
- Boiling Point [CAMEO, DRGBNK, HSDB, ICSC, NIOSH, OSHA]
- Melting Point [CAMEO, DRGBNK, HSDB, ICSC, NIOSH, OSHA]
- Flash Point [HSDB, ICSC, NIOSH, OSHA]
- Solubility [CAMEO, DRGBNK, HSDB, ICSC, NCI, NIOSH]
- Density [CAMEO, HSDB, ICSC, NIOSH, OSHA]
- Vapor Density [CAMEO, HSDB, ICSC, OSHA]
- Vapor Pressure [CAMEO, HSDB, ICSC, NIOSH, OSHA]
- Auto-Ignition [HSDB, ICSC]
- Decomposition [HSDB, ICSC]
- Corrosivity [HSDB]
- Odor Threshold [HSDB]

Toxicity Data

- Toxicity Summary [DRGBNK, HSDB]
- Human Toxicity Values [HSDB]
- Non-Human Toxicity Values [HSDB]

Exposure Limits

- Immediately Dangerous to Life or Health Concentration [NIOSH, OSHA]
- Recommended Exposure Limit (REL) [NIOSH, OSHA]
- Permissible Exposure Limit (PEL) [NIOSH, OSHA]
- REL-Time-Weighted Average Concentration (REL-TWAC) [OSHA]
- REL-Short-Term Exposure Limit (REL-STEL) [OSHA]
- REL-Ceiling (REL-C) [OSHA]
- PEL-Time-Weighted Average Concentration (PEL-TWAC) [OSHA]
- PEL-Short-Term Exposure Limit (PEL-STEL) [OSHA]
- PEL-Ceiling (PEL-C) [OSHA]
- Threshold Limit Values [HSDB]
- Occupational Exposure Limits [ICSC]
- Effects of Short Term Exposure [ICSC]
- Effects of Long Term Exposure [ICSC]
- Explosive Limits and Potential [HSDB, ICSC]
- Radiation Limits and Potential [HSDB]
- Acceptable Daily Intakes [HSDB]
- Allowable Tolerances [HSDB]

Health and Symptoms

- Symptoms [NIOSH]
- Carcinogen [ATSDR, HSDB, OSHA]
- Exposure Routes [ICSC, NIOSH]
- Target Organs [ATSDR, NIOSH]
- Cancer Sites [NIOSH]
- Fire Hazard [ICSC]
- Explosion Hazard [ICSC]
- Exposure Hazard [ICSC]
- Skin Hazard [ICSC]
- Inhalation Hazard [ICSC]
- Eye Hazard [ICSC]
- Ingestion Hazard [ICSC]
- Hazards Summary [ATSDR, EPA-AT, HSDB]
- Fire Potential [HSDB]
- Skin, Eye, and Respiratory Irritations [HSDB]

First Aid

- Fire First Aid [ICSC]
- Explosion First Aid [ICSC]
- Exposure First Aid [ICSC]
- Inhalation First Aid [ICSC]
- Skin First Aid [ICSC]
- Eye First Aid [ICSC]
- Ingestion First Aid [ICSC]

Flammability and Explosivity

- Flammability [HSDB, NIOSH]
- Lower Explosive Limit (LEL) [NIOSH, OSHA]
- Upper Explosive Limit (UEL) [NIOSH, OSHA]
- NFPA Hazard Classification [HSDB]
- NFPA Fire Rating [CAMEO, OSHA]
- NFPA Reactivity Rating [CAMEO, OSHA]
- NFPA Health Rating [CAMEO, OSHA]
- NFPA Other [CAMEO, OSHA]
- Critical Temperature [HSDB]
- Critical Pressure [HSDB]

Stability and Reactivity

- Reactivities and Incompatibilities [HSDB, NIOSH, OSHA]

Storage and Handling

- Safe Storage [ICSC]
- Storage Conditions [HSDB]
- Protective Equipment and Clothing [HSDB]
- Personal Protection [NIOSH]
- Respirator Recommendations [NIOSH]
- Nonfire Spill Response [OSHA]

Cleanup and Disposal

- Spillage Disposal [ICSC]
- Cleanup Methods [HSDB]
- Disposal Methods [HSDB]

Additional Considerations

- Toxic Combustion Products [HSDB]
- Other Hazardous Reactions [HSDB]

[http://confchem.ccce.divched.org/sites/
confchem.ccce.divched.org/files/
2015FallCCCENLP3fig5.pdf](http://confchem.ccce.divched.org/sites/confchem.ccce.divched.org/files/2015FallCCCENLP3fig5.pdf)

Access to PubChem LCSS

NIH > NLM > National Center for Biotechnology Information

PubChem OPEN CHEMISTRY DATABASE

NIH > NLM > National Center for Biotechnology Information

PubChem OPEN CHEMISTRY DATABASE

Search Compounds

Compound Summary for CID 8028

PUBCHEM > COMPOUND > TETRAHYDROFURAN > LCSS

LCSS Laboratory Chemical Safety Summary for CID 8028

Download Print Share Help

PUBCHEM > COMPOUND > TETRAHYDROFURAN > LCSS [Read about the LCSS project](#)

TETRAHYDROFURAN

Vendors Pharmacology Literature

PubChem CID: 8028

Chemical Names: TETRAHYDROFURAN; Oxolane; Furanidine; Butylene oxide; 109-99-9; Furan, tetrahydro-

Molecular Formula: C₄H₈O

Molecular Weight: 72.10572 g/mol

Cite this Record

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

1 GHS Classification

Signal: Dgr
 H225 - Highly flammable liquid and vapour
 H351 - Suspected of causing cancer
 H319 - Causes serious eye irritation
 H335 - May cause respiratory irritation

from REGULATION (EC) No 1272/2008

2 Identifiers

Tetrahydrofuran is a clear colorless liquid.

Contents

- 1 2D Structure
- 2 3D Conformer
- 3 Names and Identifiers

UNII: **Safety Summary:**

Modify Date:

Create Date:

□ Access to PubChem LCSS

The screenshot displays the PubChem website interface. At the top, there is a navigation bar with links for 'Databases >', 'Upload', 'Services >', 'Help', 'more >', and 'Today's Statistics >'. The 'Services >' link is highlighted with a red dashed box, and its dropdown menu is open. The dropdown menu contains the following items: 'BioActivity analysis >', 'Download facility >', 'Chemical structure search', 'Classification browser', 'Data Sources', 'Identifier exchange service', 'Laboratory Chemical Safety Summary' (highlighted with a red dashed box), 'PubChem3D', 'PubChemRDF', 'PUG (Power User Gateway)', 'PUG REST', 'Score matrix service', 'Standardization service', 'Structure clustering', 'Web-based 3D viewer', and 'Widgets'. To the right of the dropdown menu, there is a search bar with a 'Substance' label and a 'Go' button. Below the search bar, there is a 'Limits Advanced' link. On the right side of the page, there are social media icons for Facebook, Twitter, Google+, RSS, and a chat icon. Below these icons, there is a vertical list of services: 'BioActivity Summary', 'BioActivity Datatable', 'BioActivity SAR', 'Structure Search', '3D Conformer Tools', 'Structure Clustering', 'Classification', 'Upload', 'Download', and 'PubChem FTP'. At the bottom of the page, there is a footer with links for 'Accessibility', 'Data Citation Guidelines', 'Technology Information', and 'SIS'.

□ Access to PubChem LCSS

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



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).

PubChem
Compound

PubChem Compound

Limits Advanced

Search


Summary 20 per page Sort by Default order


Send to

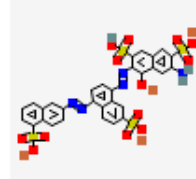
Links from pchierarchy

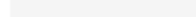
Items: 1 to 20 of 3482

<< First < Prev Page 1 of 175 Next > Last >>

1.  [Direct blue 301; 124605-82-9](#)
 MW: 1278.433288 g/mol MF: C₃₃H₂₂Li₄N₈Na₁₆O₁₄S₄
 IUPAC name: tetralithium;(3Z)-5-amino-3-[[4-[[4-[(2Z)-2-(8-amino-1-oxo-3...
 Create Date: 2016-01-08
 CID: 102601870
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#)

2.  [12427-38-2](#)
 MW: 265.301885 g/mol MF: C₄H₆MnN₂S₄
 IUPAC name: 2-(dithiocarboxyamino)ethyliminomethanedithiolate;manganese(...
 Create Date: 2015-12-27
 CID: 102460656
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#) [PubMed \(MeSH Keyword\)](#)

3.  [107246-80-0; 6-Amino-4-hydroxy-3-\[7-sulfo-4-\(5-sulfo-2-naphthylazo\)-1-naphthylazo\]-2,7-naphthalenedisulfonic acid tetralithium salt](#)
 MW: 811.505680 g/mol MF: C₃₀H₁₇Li₄N₅O₁₃S₄
 IUPAC name: tetralithium;3-amino-5-oxido-7-sulfo-6-[[7-sulfonato-4-[(5-s...
 Create Date: 2015-12-24
 CID: 102117455
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#)

 [ISODRIN; 465-73-6](#)

NIH > NLM > National Center for Biotechnology Information

Search Compounds



Compound Summary for CID 102601870



PUBCHEM > COMPOUND > DIRECT BLUE 301

Direct Blue 301

[Cite this Record](#)

Vendors



PubChem CID: 102601870

Chemical Names: Direct blue 301; 124605-82-9; [More...](#)Molecular Formula: $C_{33}H_{22}Li_4N_8Na_{10}O_{14}S_4$

Molecular Weight: 1278.433288 g/mol

InChI Key: DLNIVGKCMNJVK-VVOGLQFISA-J

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

Modify Date: 2016-03-15

Create Date: 2016-01-08

[+ Contents](#)

1 2D Structure



Direct Blue 301

[Cite this Record](#)



PubChem CID:	102601870
Chemical Names:	Direct blue 301; 124605-82-9
Molecular Formula:	C ₃₃ H ₂₂ Li ₄ N ₈ Na ₁₆ O ₁₄ S ₄
Molecular Weight:	1278.433288 g/mol

Contents

- 1 GHS Classification
- 2 Identifiers
 - 2.1 InChI
 - 2.2 InChI Key
- 3 Information Sources

1 GHS Classification



Signal: **Warning**

GHS Hazard Statements

H317: May cause an allergic skin reaction [**Warning** Sensitization, Skin - Category 1]
 H411: Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard - Category 2]

Precautionary Statements

□ Access to PubChem LCSS

➤ Classification Browser

[\(https://pubchem.ncbi.nlm.nih.gov/classification\)](https://pubchem.ncbi.nlm.nih.gov/classification)

- Browse PubChem data using a classification of interest.
- Search for records annotated with the desired classification/term.
- Current available ontologies/classifications.
 - MeSH
 - ChEBI
 - FDA Pharm Classes
 - KEGG
 - LIPID MAPS classification system for lipids
 - PubChem Compound Table of Contents
 - PubChem BioAssay Classification
 - WHO ATC Code (Anatomical Therapeutic Chemical Classification System)
 - WIPO International Patent Classification 2014

The screenshot displays the PubChem website interface. At the top, navigation tabs include 'Databases', 'Upload', 'Services', 'Help', 'more', and 'Today's Statistics'. The 'Services' dropdown menu is open, listing various tools such as 'BioActivity analysis', 'Download facility', 'Chemical structure search', 'Classification browser', 'Data Sources', 'Identifier exchange service', 'Laboratory Chemical Safety Summary', 'PubChem3D', 'PubChemRDF', 'PUG (Power User Gateway)', 'PUG REST', 'Score matrix service', 'Standardization service', 'Structure clustering', 'Web-based 3D viewer', and 'Widgets'. The 'Classification browser' option is highlighted with a red dashed box. In the top right corner, there are social media icons for Facebook, Twitter, Google+, RSS, and a chat icon. Below these icons is a sidebar of tool buttons: 'BioActivity Summary', 'BioActivity Datable', 'BioActivity SAR', 'Structure Search', '3D Conformer Tools', 'Structure Clustering', 'Classification', 'Upload', 'Download', and 'PubChem FTP'. The 'Classification' button is also highlighted with a red dashed box. The main content area features a search bar with a 'Substance' label, a 'Go' button, and a 'Limits Advanced' link. A notification banner at the bottom states 'New Substance databases is available.' with a 'more...' link and an RSS icon. Footer links include 'Accessibility', 'Data Citation Guidelines', 'Technology Information', and 'SIS'.

Access to PubChem LCSS

NCBI

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; Ontology: DNA repair). [More...](#)

1

Select classification: **PubChem** 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 2015/08/06.
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, Substance Categorization Classification, Computed Descriptors, Deleted Synonyms, Supplied Synonyms, Removed Synonyms, Create Date, Modify Date, Record Title, Related Compounds, Related Compounds with Annotation, Related Instances, 2D Structure, 3D Conformer, and Chemical Vendors. [More...](#)

2

Data type counts to display: **Compound** Display zero count nodes? **Yes** **No** Filter by Entrez History: Choose one

Browse PubChem Tree

- ▼ PubChem Compound TOC ? 23,173,396
 - ▶ Biologic Description ?
 - ▶ Biological Test Results ? 2,090,746
 - ▶ Biomolecular Interactions and Pathways ? 42,495
 - ▶ Chemical and Physical Properties ? 54,268

PubChem
Compound

PubChem Compound

Limits Advanced

Search

Summary 20 per page Sort by Default order

Send to

Links from pchierarchy

Items: 1 to 20 of 3482

<< First < Prev Page 1 of 175 Next > Last >>

1.



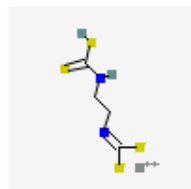
[Direct blue 301; 124605-82-9](#)

MW: 1278.433288 g/mol MF: C₃₃H₂₂Li₄N₈Na₁₆O₁₄S₄
IUPAC name: tetralithium;(3Z)-5-amino-3-[[4-[[4-[(2Z)-2-(8-amino-1-oxo-3...
Create Date: 2016-01-08

CID: 102601870

[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#)

2.



[12427-38-2](#)

MW: 265.301885 g/mol MF: C₄H₆MnN₂S₄
IUPAC name: 2-(dithiocarboxyamino)ethyliminomethanedithiolate;manganese(...
Create Date: 2015-12-27

CID: 102460656

[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#) [PubMed \(MeSH Keyword\)](#)

3.



[107246-80-0; 6-Amino-4-hydroxy-3-\[7-sulfo-4-\(5-sulfo-2-naphthylazo\)-1-naphthylazo\]-2,7-naphthalenedisulfonic acid tetralithium salt](#)

MW: 811.505680 g/mol MF: C₃₀H₁₇Li₄N₅O₁₃S₄
IUPAC name: tetralithium;3-amino-5-oxido-7-sulfo-6-[[7-sulfonato-4-[(5-s...
Create Date: 2015-12-24

CID: 102117455

[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#)

[ISODRIN; 465-73-6](#)

□ Access to PubChem LCSS

- PubChem LCSS data are downloadable in XML, JSON, & ASN.1
- Bulk download via FTP
(<ftp://ftp.ncbi.nlm.nih.gov/pubchem/Compound/Extras/CID-LCSS.xml.gz>)
- Additional PubChem data are available
(through programmatic access route called PUG-REST)

Customization of LCSS

for specific procedures at individual institutions

□ Limitations

- PubChem aggregates data from multiple sources without thorough accuracy check
→ Users need to review the accuracy and variability of data
- Ambiguity in name-structure associations
formaldehyde vs. formalin (saturated water solution)
- Different units, precisions, and measurement conditions

□ Limitations

Different units

Different conditions & precisions

Naphtha (coal tar)

Mixture of Benzene, toluene & xylenes

4.2.5 Boiling Point ?

80.08 deg C
Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 94th Edition. CRC Press LLC, Boca Raton: FL 2013-2014, p. 3-34

▶ from HSDB

80°C

▶ from ILO-ICSC

176°F

▶ from NIOSH-PocketGuide, OSHA Occupational Chemical DB

320-428°F

▶ from NIOSH-PocketGuide, OSHA Occupational Chemical DB

176.2 °F (at 760 mmHg)
(NTP, 1992)

▶ from CAMEO Chemicals

200 to 500 °F (at 760 mmHg)
(USCG, 1999)

▶ from CAMEO Chemicals

230 to 374°F

▶ from OSHA Chemical Sampling Information

□ Comparison between data sources

- GHS information is from four different sources.
 - EU Regulation
 - ILO
 - Japanese NITE
 - Safe Work Australia

Sometimes they provide very different GHS information

Databases > Upload Services > Help more > Today's Statistics >



PubChem

BioAssay Compound Substance

[Limits](#) [Advanced](#)

Try the new [PubChem Search](#)

New PubChem presents at the 251st American Chemical Society National Meeting in San Diego (March 13-17, 2016). Read more at <http://1.usa.gov/1QBp0aE>

New A new article about the PubChem Compound and Substance databases is available. [Read more...](#)

[more ...](#)

- [BioAssay Tools](#)
- [Structure Search](#)
- [3D Conformer Tools](#)
- [Structure Clustering](#)
- [Classification](#)
- [Upload](#)
- [Download](#)
- [PubChem FTP](#)

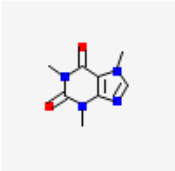
PubChem Compound PubChem Compound caffeine Search

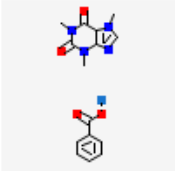
Create alert Limits Advanced Help

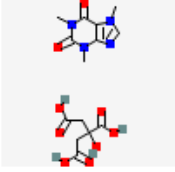
Summary 20 per page Sort by Default order Send to Filters: Manage Filters

Search results

Items: 1 to 20 of 226 << First < Prev Page 1 of 12 Next > Last >>

1.  **caffeine; Methyltheobromine; Guanine ...**
 MW: 194.190600 g/mol MF: C₈H₁₀N₄O₂
 IUPAC name: 1,3,7-trimethylpurine-2,6-dione
 Create Date: 2004-09-16
 CID: 2519
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#) [PubMed \(MeSH Keyword\)](#) Active in 124 of 2792 BioAssays

2.  **Caffeine sodium benzoate; Sodium caffeine benzoate; Annaca ...**
 MW: 338.293769 g/mol MF: C₁₅H₁₅N₄NaO₄
 IUPAC name: sodium;1,3,7-trimethylpurine-2,6-dione;benzoate
 Create Date: 2008-02-05
 CID: 23669229
[Summary](#) [Similar Compounds](#) [Mixture/Component Compounds](#)

3.  **Caffeine citrate; Caffeine, Citrated; 69-22-7 ...**
 MW: 386.314120 g/mol MF: C₁₄H₁₈N₄O₉
 IUPAC name: 2-hydroxypropane-1,2,3-tricarboxylic acid;1,3,7-trimethylpur...
 Create Date: 2005-03-26
 CID: 6241
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#) [PubMed \(MeSH Keyword\)](#) Active in 1 of 148 BioAssays

- 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 (144)
- BioActivity Experiments**
- BioAssays, Active (73)
 - BioAssays, Tested (109)
 - Protein 3D Structures (2)
 - Thermostabilised Adenosine A2a Receptor In Complex With Caffeine (1)
 - Crystal Structure Of A Chitinase Crchi1 From The Nematophagous Fungus

NIH > NLM > National Center for Biotechnology Information

Search Compounds



Compound Summary for CID 2519

Download

Print

Help

PUBCHEM > COMPOUND > CAFFEINE

Caffeine

[▶ Cite this Record](#)

Vendors



Drug Information



Pharmacology



Literature



Patents



Bioactivities



PubChem CID:	2519
Chemical Names:	Caffeine; Methyltheobromine; Guanine; 1,3,7-Trimethylxanthine; Cafeina; Koffein; More...
Molecular Formula:	$C_8H_{10}N_4O_2$
Molecular Weight:	194.1906 g/mol
InChI Key:	RYYVLZVUVIJVGH-UHFFFAOYSA-N
Safety Summary:	Laboratory Chemical Safety Summary (LCSS)
Modify Date:	2016-03-15
Create Date:	2004-09-16



Caffeine

[Cite this Record](#)

PubChem CID: 2519

Chemical Names: Caffeine; Methyltheobromine; Guaranine; 1,3,7-Trimethylxanthine; Cafeina; Koffein

Molecular Formula: $C_8H_{10}N_4O_2$

Molecular Weight: 194.1906 g/mol

+ Contents

[1 GHS Classification](#)[2 Identifiers](#)[3 Physical Properties](#)[4 Toxicity Data](#)[5 Exposure Limits](#)[6 Health and Symptoms](#)[7 First Aid](#)[8 Storage and Handling](#)[9 Cleanup and Disposal](#)[10 Additional Considerations](#)[11 Information Sources](#)

1 GHS Classification

Signal: **Warning**

GHS Hazard Statements

H302: Harmful if swallowed [**Warning** Acute toxicity, oral - Category 4]

Precautionary Statements

P264: Wash ... thoroughly after handling.

P270: Do not eat, drink or smoke when using this product.

P301+P312: IF SWALLOWED: call a POISON CENTER/doctor/... IF you feel unwell.

P330: Rinse mouth.

P501: Dispose of contents/container to ...

[from EU REGULATION \(EC\) No 1272/2008](#)[View GHS Classification from all \(3\) sources.](#)

PUBCHEM > COMPOUND > CAFFEINE > SAFETY-AND-HAZARDS > HAZARDS-IDENTIFICATION > GHS-CLASSIFICATION

Caffeine

GHS Classification ?



Signal: [Warning](#)

GHS Hazard Statements

H302: Harmful if swallowed [[Warning](#) Acute toxicity, oral - Category 4]

Precautionary Statements

P264: Wash ... thoroughly after handling.

P270: Do not eat, drink or smoke when using this product.

P301+P312: IF SWALLOWED: call a POISON CENTER/doctor/... IF you feel unwell.

P330: Rinse mouth.

P501: Dispose of contents/container to ...

▶ from EU REGULATION (EC) No 1272/2008, Safe Work Australia - HSIS

EU & Australia provided the same information on caffeine



Signal: **Danger**

GHS Hazard Statements

H301: Toxic if swallowed [**Danger** Acute toxicity, oral - Category 3]

H332: Harmful if inhaled [**Warning** Acute toxicity, inhalation - Category 4]

H360: May damage fertility or the unborn child [**Danger** Reproductive toxicity - Category 1A, 1B]

H402: Harmful to aquatic life [Hazardous to the aquatic environment, acute hazard - Category 3]

H412: Harmful to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard - Category 3]

Precautionary Statements

P201: Obtain special instructions before use.

P202: Do not handle until all safety precautions have been read and understood.

P261: Avoid breathing dust/fume/gas/mist/vapors/spray.

P264: Wash ... thoroughly after handling.

P270: Do not eat, drink or smoke when using this product.

P271: Use only outdoors or in a well-ventilated area.

P273: Avoid release to the environment.

P281: Use personal protective equipment as required.

P301+P310: IF SWALLOWED: Immediately call a POISON CENTER/doctor/...

P304+P312: IF INHALED: Call a POISON CENTER/doctor/... if you feel unwell.

P304+P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P308+P313: IF exposed or concerned: Get medical advice/attention.

P312: Call a POISON CENTER or doctor/... if you feel unwell.

P321: Specific treatment (see ... on this label).

P330: Rinse mouth.

P405: Store locked up.

P501: Dispose of contents/container to ...

▸ from NITE-CMC

Japan's GHS classifications are very different.



Signal: **Danger**

GHS Hazard Statements

- H301: Toxic if swallowed [**Danger** Acute toxicity, oral - Category 3]
H332: Harmful if inhaled [**Warning** Acute toxicity, inhalation - Category 4]
H360: May damage fertility or the unborn child [**Danger** Reproductive toxicity - Category 1A, 1B]
H402: Harmful to aquatic life [Hazardous to the aquatic environment, acute hazard - Category 3]
H412: Harmful to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard - Category 3]

Precautionary Statements

- P201: Obtain special instructions before use.
P202: Do not handle until all safety precautions have been read and understood.
P261: Avoid breathing dust/fume/gas/mist/vapors/spray.
P264: Wash ... thoroughly after handling.
P270: Do not eat, drink or smoke when using this product.
P271: Use only outdoors or in a well-ventilated area.
P273: Avoid release to the environment.
P281: Use personal protective equipment as required.
P301+P310: IF SWALLOWED: Immediately call a POISON CENTER/doctor/...
P304+P312: IF INHALED: Call a POISON CENTER/doctor/... if you feel unwell.
P304+P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P308+P313: IF exposed or concerned: Get medical advice/attention.
P312: Call a POISON CENTER or doctor/... if you feel unwell.
P321: Specific treatment (see ... on this label).
P330: Rinse mouth.
P405: Store locked up.
P501: Dispose of contents/container to ...

▼ from NITE-CMC

Source Name: NITE-CMC

Record Name: caffeine

URL: <http://www.safe.nite.go.jp/english/ghs/08-mhlw-0136e.html>

Description: The chemical classification in this section was conducted by the Chemical Management Center (CMC) of Japan National Institute of Technology and Evaluation (NITE) in accordance with GHS Classification Guidance for the Japanese Government, and is intended to provide a reference for preparing GHS labelling and SDS for users.

GHS Classification Result

Chemical Name: caffeine

CAS:58-08-2

Result :

ID: 20A2140

Classifier: Ministry of Health, Labour and Welfare (MHLW), Ministry of the Environment (MOE)


Year Classified: FY2008

Reference: GHS Classification Guidance by the Japanese Government (Sep, 2008)

Manual:

PHYSICAL HAZARDS

	Hazard class	Classification	Symbol	Signal word	Hazard statement	Precautionary statement	Rationale for the classification
1	Explosives	Not applicable	-	-	-	-	There are no chemical groups associated with explosive properties present in the molecules.
2	Flammable gases (including chemically unstable gases)	Not applicable	-	-	-	-	Solid (GHS definition)
3	Aerosols	Not applicable	-	-	-	-	Not aerosol products.
4	Oxidizing gases	Not applicable	-	-	-	-	Solid (GHS definition)
5	Gases under pressure	Not applicable	-	-	-	-	Solid (GHS definition)
6	Flammable liquids	Not applicable	-	-	-	-	Solid (GHS definition)
7	Flammable solid	Classification not possible	-	-	-	-	No data available.
8	Self-reactive substances and mixtures	Not applicable	-	-	-	-	There are no chemical groups present in the molecule associated with explosive or self-reactive properties.
9	Pyrophoric liquids	Not applicable	-	-	-	-	Solid (GHS definition)
10	Pyrophoric solids	Not classified	-	-	-	-	Its autoignition point is 540degC (IUCILID (2000)),

Symbol	Signal word	Hazard statement	Precautionary statement	Rationale for the classification
	Danger	H301: Toxic if swallowed	P301+P310: IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician. P264: Wash ... thoroughly after handling. P270: Do not eat, drink or smoke when using this product. P321: Specific treatment (see ... on this label). P330: Rinse mouth. P405: Store locked up. P501: Dispose of contents/container to ...	Since its twelve LD50 values for rats (261 – 383, 200 – 400, 192, 483, 233, 355, 247, 344, 421, 700, 50 – 500, and 261 – 383 mg/kg) have been reported in List 1 literature, and seven of them are within the guidance values of Category 3 and five Category 4 (SIDS (accessed in September 2008)), the substance was classified into Category 3.
	Vapours)	not possible		
				P304+P340: IF INHALED: Remove victim to fresh air

□ Summary

- PubChem LCSS is a concise view of health and safety information for a given compound
- Data are collected from many authoritative sources.
- Available to the public free of charge.
- Can be downloaded and annotated for customization.
- PubChem is actively collecting more GHS data to increase the LCSS coverage.

Thank you!