

2019 Fall ACS National Meeting in San Diego
August 26, 2019

PubChem LCSS (Laboratory Chemical Safety Summary)

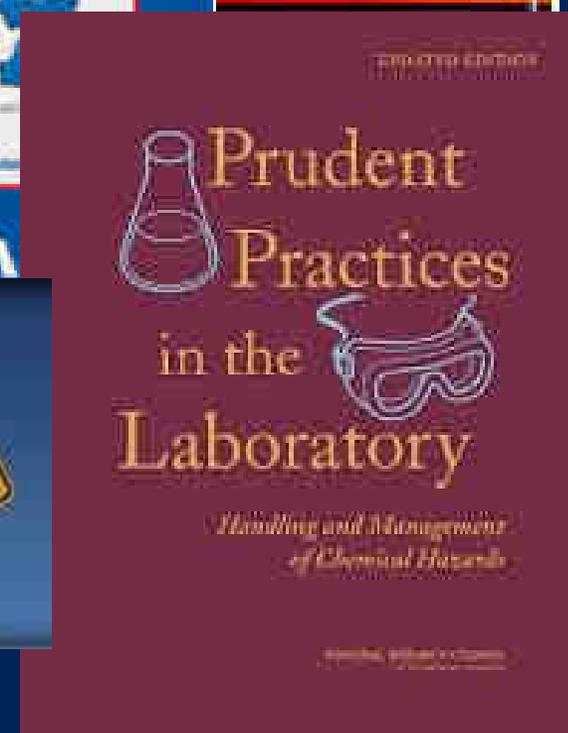
Jian Zhang*, Paul Thiessen, Asta Gindulyte, Evan Bolton,
Leah McEwen, Ralph Stuart



U.S. National Library of Medicine
National Center for Biotechnology Information

Lab Safety ...

- .. an important and fundamental topic in chemistry labs
- .. safety guidelines in every lab
- .. chemical safety handbooks ..
- .. accidents occurred from time to time



LCSS - Laboratory Chemical Safety Summary

• LCSS

ACETALDEHYDE

SYNONYMS	CAS#	Formula
Ethanal, acetic aldehyde, ethyl aldehyde	75-07-0	<chem>CC=O</chem>

PHYSICAL PROPERTIES

Odor:	Pungent, fruity odor detectable at 0.0068 to 1,000 ppm (mean = 0.067 ppm)	Appearance:	Clear, colorless
Water Solubility:	Miscible with water	Vapor Density:	1.52 (air = 1.0)
Flash Point:	-27 °C	Vapor Pressure:	740 mmHg at 20 °C
Autoignition:	140 °C	bp/mp:	21 °C/-124 °C

TOXICITY

EXPOSURE LIMITS	
LD₅₀ oral (rat):	661 mg/kg
TLV-TWA	100 ppm (180 mg/m ³)
LC₅₀ inha	270 mg/m ³
LC₅₀ skin	360 mg/m ³

HEALTH

General

Accidental exposure can produce symptoms similar to alcoholism.

Skin Causes irritation and burning upon skin contact

Eyes Severe eye irritant

Ingestion May cause severe irritation of the digestive tract leading to nausea, vomiting, headache, and liver damage.

Inhalation

FIRST AID

Skin

Eyes

Ingestion

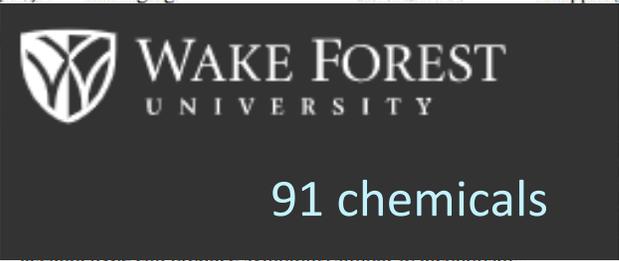
Inhalation

FLAMMABLE

Extremely flammable

NFPA

Use carbon dioxide or dry chemical extinguishers. Explosive vapors in air can be ignited by surfaces such as hot plates or lightbulbs, or by static electricity discharges. The vapor is heavier than air and may travel a considerable distance to an ignition source and flash back.



LABORATORY CHEMICAL SAFETY SUMMARY: ACETIC ACID

Substance Acetic acid (Ethanoic acid)
CAS 64-19-7

Formula CH₃COOH

Physical Properties Colorless liquid
bp 118 °C, mp 17 °C
Miscible in water (100 g/100 mL)

Odor Strong, pungent, vinegar-like odor detectable at 0.2 to 1.0 ppm

Vapor Density 2.1 (air = 1.0)

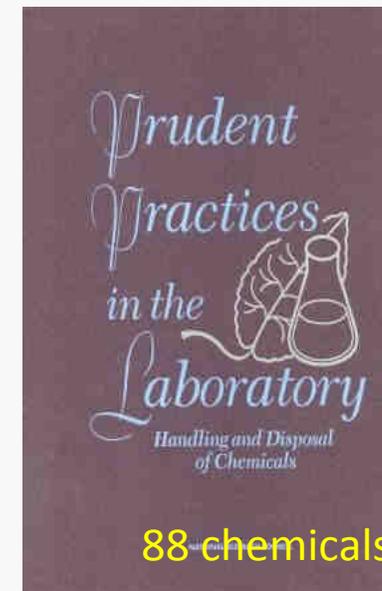
Vapor Pressure 11 mmHg at 20 °C

Flash Point 39 °C

Autoignition 426 °C

Temperature

Toxicity Data LD₅₀ oral (rat)
LD₅₀ skin (rabbit)
LC₅₀ inhal (mice)
PEL (OSHA)
TLV-TWA (ACGIH)
STEL (ACGIH)



Needs for online resource for chemical safety information

LCSS - Laboratory Chemical Safety Summary

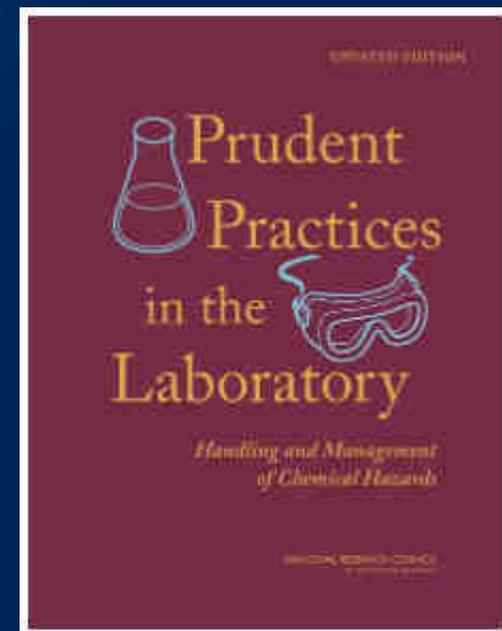
In 2015, PubChem, together with health and safety professionals from CHAS, CINF, and universities, created an online version of LCSS. With several updates, the current PubChem LCSS is fully digitized and the data behind is fully machine readable.

Outline ..

- PubChem LCSS overview
- LCSS content
- LCSS updates
- LCSS data access and retrieval
- Summary

LCSS - Laboratory Chemical Safety Summary

- Subset of the PubChem compound summary
- Format of TOC - Prudent Practices in the Laboratory: Handling and Management of Chemical Hazards (2011) + GHS + ...



Data ... chemical centralized and beyond

- Chemical structure — 2D/3D, SMILES, InChI, SDF..
 - Property -
 - Drug and medication
 - Agrochemicals
 - Food additives
 - Safety and hazards
 - Toxicity
 - Literature
 - Patents
 - Bioactivity
 - Target
 - Natural products
 - Pathways
 - ... more
-
- ```
graph LR; A[Property -] --> LCSS[LCSS]; B[Safety and hazards] --> LCSS; C[Toxicity] --> LCSS;
```

# PubChem LCSS Contents

- Example: Acetone

1. Google/PubChem search ... acetone
2. Launch the PubChem acetone page
3. Click the LCSS link

# PubChem LCSS - acetone

PubChem About Blog Submit Contact

Search PubChem em

COMPOUND SUMMARY > LABORATORY CHEMICAL SAFETY SUMMARY (LCSS)

## Acetone

PubChem CID: 180

Structure:  2D  
[Find Similar Structures](#)

Molecular Weight: 58.08 g/mol

[Learn More About LCSS Project >](#)

### 1 GHS Classification

Showing 1 of 5 [View More](#)

|              |                                                                                                                                                                             |
|--------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Pictogram(s) |   |
| Signal       | <b>Danger</b>                                                                                                                                                               |

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Cite Download

CONTENTS

- Title and Summary
- 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 Information Sources

<https://pubchem.ncbi.nlm.nih.gov/compound/Acetone#datasheet=LCSS>

# PubChem LCSS Contents

- 12 main headings
- Each section may have multiple subheadings
- Each data item may have multiple values integrated from multiple sources.

# PubChem LCSS Contents

|                                |   |
|--------------------------------|---|
| CONTENTS                       | ^ |
| Title and Summary              |   |
| 1 GHS Classification           |   |
| 2 Identifiers                  | ▼ |
| 3 Physical Properties          | ▼ |
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| 5 Exposure Limits              | ▼ |
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| 9 Stability and Reactivity     | ▼ |
| 10 Storage and Handling        | ▼ |
| 11 Cleanup and Disposal        | ▼ |
| 12 Information Sources         |   |

|                               |   |
|-------------------------------|---|
| 2 Identifiers                 | ▼ |
| 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 Autoignition Temperature |   |
| 3.11 Odor Threshold           |   |
| 4 Toxicity Data               | ▼ |
| 5 Exposure Limits             | ▼ |
| 6 Health and Symptoms         | ▼ |

# PubChem LCSS – Total LCSSs

- More than 120

- 2015 – 3,000

- 2017 – 5,000

- 2018 – 108,000

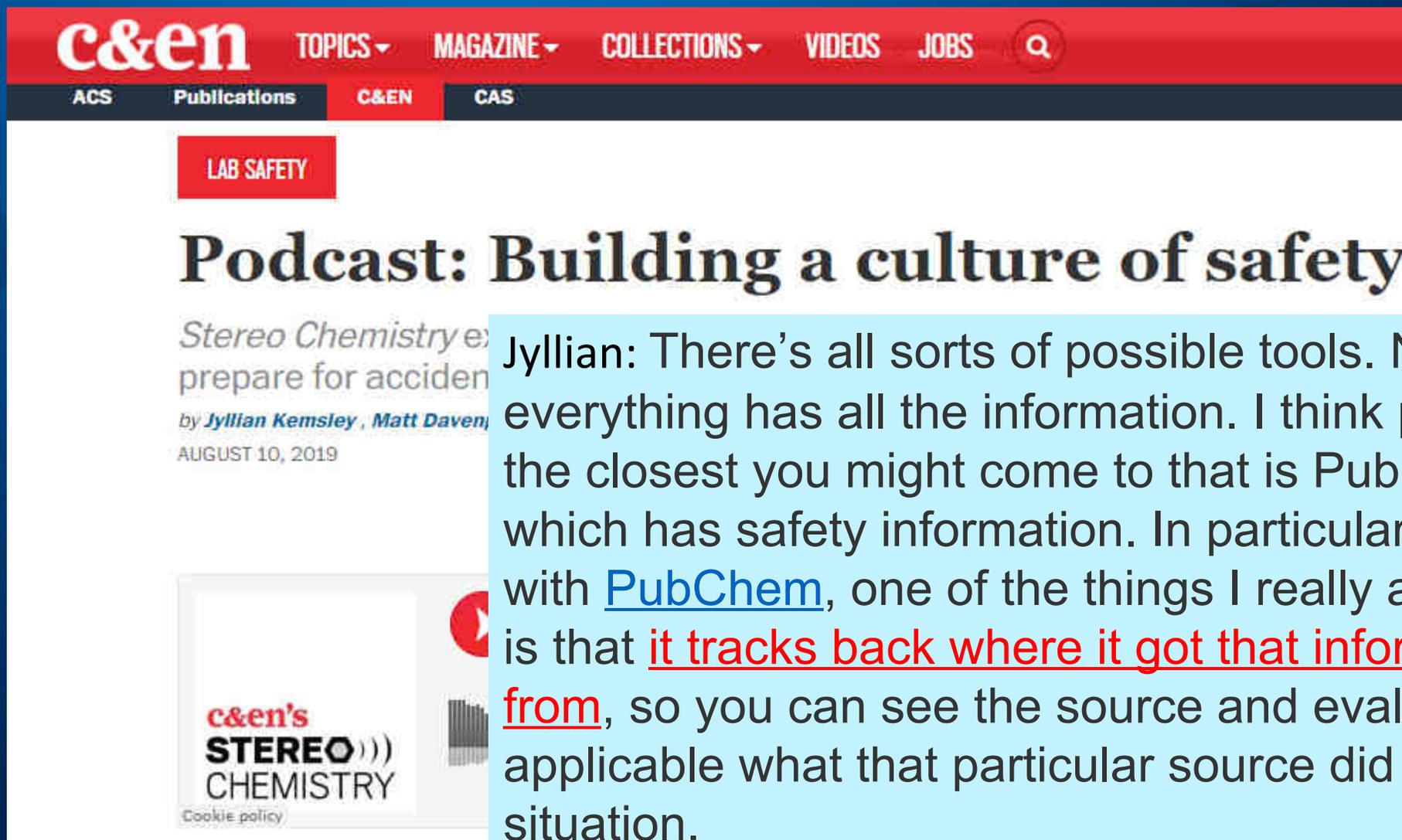
- 2019 – 122,000

## Browse PubChem: PubChem Compound TOC Tree

- PubChem Compound TOC ? 32,590,514
  - Agrochemical Information ? 1,995
  - Biologic Description ? 538,464
  - Biological Test Results ? 3,460,759
  - Biomolecular Interactions and Pathways ? 59,555
  - Chemical and Physical Properties ? 237,692
  - Classification ? 18,237,311
  - Drug and Medication Information ? 15,858
  - Food Additives and Ingredients ? 7,431
  - Identification ? 5,699
  - Information Sources ? 20,292,987
  - Literature ? 1,661,748
  - Names and Identifiers ? 1,306,374
  - Patents ? 21,676,810
  - Pharmacology and Biochemistry ? 123,740
  - Related Records ? 5,208,345
  - Safety and Hazards ? 124,660
  - Spectral Information ? 761,299
  - Structures ? 5,875,987
  - Toxicity ? 114,476
  - Use and Manufacturing ? 108,481
- Chemical Safety ? 121,971
- Preferred Compound ?

- Related Records ? 5,208,345
- Safety and Hazards ? 124,660
  - Accidental Release Measures ? 8,758
  - Exposure Control and Personal Protection ? 7,404
  - Fire Fighting ? 6,556
  - First Aid Measures ? 5,147
  - Handling and Storage ? 7,569
  - Hazards Identification ? 123,264
    - CLP Hazard Class and Category Codes ?
    - EPA Hazardous Waste Number 753
    - EPA Safer Chemical ? 871
    - Explosion Hazard ?
    - Fire Hazard ? 5,065
    - Fire Potential ? 1,952
    - [REDACTED]
    - Hazards Summary ? 372
    - Health Hazard ? 4,407
    - Skin, Eye, and Respiratory Irritations ? 2,607
  - Other Safety Information ? 4,474
  - Regulatory Information ? 5,633
  - Safety and Hazard Properties ? 2,396
  - Stability and Reactivity ? 4,843
  - Transport Information ? 4,179
- Spectral Information ? 761,299
- Structures ? 5,875,987

# Online resources for the Culture of Safety



The screenshot shows the top navigation bar of the c&en website with links for TOPICS, MAGAZINE, COLLECTIONS, VIDEOS, and JOBS. Below this is a secondary navigation bar with ACS, Publications, C&EN, and CAS. A red box labeled 'LAB SAFETY' is positioned above the main article title. The article title is 'Podcast: Building a culture of safety'. Below the title, the text reads 'Stereo Chemistry episode 10: how to prepare for accidents' by Jyllian Kemsley and Matt Davenport, dated August 10, 2019. A small image of the podcast cover is visible at the bottom left of the article area.

Jyllian: There's all sorts of possible tools. Not everything has all the information. I think possibly the closest you might come to that is PubChem, which has safety information. In particular with [PubChem](#), one of the things I really appreciate is that it tracks back where it got that information from, so you can see the source and evaluate how applicable what that particular source did is to your situation.

# LCSS Data and Provenance

- LCSS data are integrated from many sources
- The data source link allows users to track back the original data site.

E.g. GHS for toluene:

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



# PubChem GHS Summary

## GHS Classification

GHS, the 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. This page summarizes the relationship of GHS hazard statements, pictograms, signal words, hazard classes, categories, and precautionary statements.

Ref: UNECE GHS (Rev.7) (2017)

[Hazard Class Pictograms](#)

[GHS Hazard Statements](#)

[EU Hazard Statements](#)

[SWA Hazard Statements](#)

[Precautionary Statements](#)

## Hazard Class Pictograms



Explosive 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

Note: All pictograms are shown in svg format in the page. The corresponding gif images are also available, e.g. <https://pubchem.ncbi.nlm.nih.gov/images/ghs/GHS08.gif>

## GHS Hazard Statements

# LCSS Updates

- Webpage layout (look and feel).
- Backend data: the backend data format has a significant change.
- Reduced the page size for default display:
  - A LCSS page showing only 1 or 2 values for most data headings, users can view additional values by click expand icon.
- Added reactivity alerts.
- Added NFPA 704 diamond.
- Added GHS “not classified” category

# LCSS webpage updates – Look and Feel

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

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Search PubChem

LCSS Laboratory Chemical Safety Summary for CID 180

## Acetone

PubChem CID: 180  
Chemical Names: Acetone; 2-propanone; Propanone; 67-64-1; Dimethyl ketone; Methyl ketone  
Molecular Formula: C<sub>3</sub>H<sub>6</sub>O; CH<sub>3</sub>-CO-CH<sub>3</sub>  
Molecular Weight: 58.08 g/mol

PUBCHEM > COMPOUND > ACETONE > LCSS

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### 1 GHS Classification

**Signal:** Danger  
**GHS Hazard Statements**  
H225: Highly Flammable liquid and vapor [Danger]  
H319: Causes serious eye irritation [Warning] Ser  
H336: May cause drowsiness or dizziness [Warning]

**Precautionary Statement Codes**  
P210, P233, P240, P241, P242, P243, P261, P264, P337+P313, P370+P378, P403+P233, P403+P23  
(The corresponding statement to each P-code c

## Acetone

COMPOUND SUMMARY > LABORATORY CHEMICAL SAFETY SUMMARY (LCSS)

PubChem CID: 180

Structure:  2D

[Find Similar Structures](#)

**Chemical Names:** acetone, 2-propanone, propanone, 67-64-1, Dimethyl ketone, [More...](#)

**Molecular Formula:** C<sub>3</sub>H<sub>6</sub>O or CH<sub>3</sub>-CO-CH<sub>3</sub> or CH<sub>3</sub>COCH<sub>3</sub>

**Molecular Weight:** 58.08 g/mol

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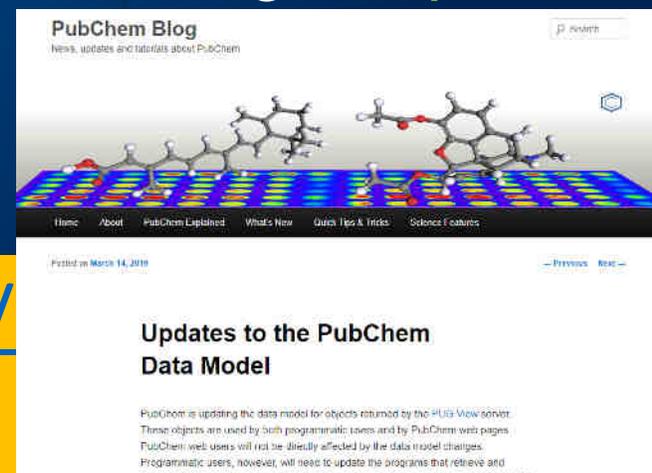
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# LCSS Updates – Backend data

- No more HTML markup within strings, instead, we have an explicit markup object that separates primary strings from the various markup types. No more embedded tables in the data blobs.
- All HTML entities are replaced by UTF-8 characters, e.g. `&alpha;` `&#945;` or `&#x3B1;`  $\rightarrow$   $\alpha$ .

<https://pubchemblog.ncbi.nlm.nih.gov/2019/the-pubchem-data-model/>



# LCSS Updates – Backend data spec

- Data blob specification

- [https://pubchem.ncbi.nlm.nih.gov/pug\\_view](https://pubchem.ncbi.nlm.nih.gov/pug_view)

```
<?xml version="1.0" encoding="UTF-8" ?>
<xs:schema xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns="http://pubchem.ncbi.nlm.nih.gov/pug_view"
targetNamespace="http://pubchem.ncbi.nlm.nih.gov/pug_view" elementFormDefault="qualified" attributeFormDefault="unqualified">
 <!--.....-->
 <xs:element name="Fault">...</xs:element>
 <xs:element name="Records">...</xs:element>
 <xs:element name="Record">...</xs:element>
 <xs:element name="Section">...</xs:element>
 <xs:element name="Information">...</xs:element>
 <!--
 Value and stringWithMarkup must be the same as in annotations_3.xsd
 -->
 <xs:element name="Value">
 <xs:complexType>
 <xs:sequence>
 <xs:choice>
 <xs:element name="Number" type="xs:double" maxOccurs="unbounded"/>
 <xs:element name="DateISO8601" type="xs:string" maxOccurs="unbounded"/>
 <xs:element name="Boolean" type="xs:boolean" maxOccurs="unbounded"/>
 <xs:element ref="StringWithMarkup" maxOccurs="unbounded"/>
 <xs:element name="Binary" type="xs:base64Binary" maxOccurs="unbounded"/>
 <xs:element name="BinaryToStore" type="xs:base64Binary" maxOccurs="unbounded"/>
 <xs:element name="ExternalDataURL" type="xs:string" maxOccurs="unbounded"/>
 <xs:element name="ExternalTableName" type="xs:string"/>
 </xs:choice>
 <xs:element name="Unit" type="xs:string" minOccurs="0"/>
 <xs:element name="MimeType" type="xs:string" minOccurs="0"/>
 <xs:element name="ExternalTableNumRows" type="xs:int" minOccurs="0"/>
 </xs:sequence>
 </xs:complexType>
 </xs:element>
 <xs:element name="StringWithMarkup">...</xs:element>
 <!-- DisplayControls must be the same as in toc_3.xsd -->
 <xs:element name="DisplayControls">...</xs:element>
 <xs:element name="Reference">...</xs:element>
 <!-- specialized containers -->
 <xs:element name="Neighbors">...</xs:element>
 <xs:element name="Structure">...</xs:element>
 <xs:element name="SourceCategories">...</xs:element>
 <xs:element name="Literature">...</xs:element>
 <xs:element name="Linkout">...</xs:element>
 <xs:element name="Reactions">...</xs:element>
</xs:schema>
```



# LCSS Updates – Page size reduced

PUBCHEM > ACETONE > LABORATORY CHEMICAL SAFETY SUMMARY (LCSS) > BOILING POINT

CID 180

## Acetone

### Boiling Point



133 ° F at 760 mm Hg (NTP, 1992)

*National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.*

▶ from CAMEO Chemicals

55.75°C

▶ from EPA DSSTox

56.08 deg C

*Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-4*

▶ from HSDB

56 °C

▶ from ILO-ICSC

133°F

▶ from OSHA Occupational Chemical DB; The National Institute for Occupational Safety and Health (NIOSH)

# LCSS Updates – reactivity alerts

## 9.3 Reactivity Alerts

Highly Flammable

▶ from CAMEO Chemicals

### 9.3.1 CSL Reaction Information

Showing 2 of 8 View More

|                    |                                               |
|--------------------|-----------------------------------------------|
| CSL No             | CSL00003                                      |
| Reactants/Reagents | ACETONE; sodium percarbonate                  |
| Reaction Class     | oxidation                                     |
| GHS Category       | Explosive                                     |
| Reaction Scale     | S (up to 1g)                                  |
| Warning Message    | can form explosive acetone peroxide compounds |
| Source Reference   | User-Reported                                 |
| CSL Status         | Approved                                      |
| Additional Info    | Bassan et al OPRD 2013, 17, 1611-1616         |
| Modified Date      | 2/27/2018                                     |

▶ from Pistoia Alliance Chemical Safety Library

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9 Stability and Reactivity

9.1 Hazardous Reactivities & Incompatibilities

9.2 Reactivity Profile

9.3 Reactivity Alerts

9.3.1 CSL Reaction Information

10 Storage and Handling

# LCSS Updates – NFPA 704 Diamond

## 8.4 NFPA Hazard Classification



Showing 1 of 2 [View More](#)

|                         |                                                                                                                                                                                                                                                                                    |
|-------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| NFPA 704 Diamond        | <br>1-3-0                                                                                                                                                                                        |
| NFPA Health Rating      | 1 - Materials that, under emergency conditions, can cause significant irritation.                                                                                                                                                                                                  |
| NFPA Fire Rating        | 3 - Liquids and solids that can be ignited under almost all ambient temperature conditions. Materials produce hazardous atmospheres with air under almost all ambient temperatures or, though unaffected by ambient temperatures, are readily ignited under almost all conditions. |
| NFPA Instability Rating | 0 - Materials that in themselves are normally stable, even under fire conditions.                                                                                                                                                                                                  |

▶ from HSDB

# LCSS Updates – GHS “not classified”

## Summary of Classification and Labelling

### Notified classification and labelling

#### General Information

| EC / List no.<br>? | Name  | CAS Number<br>? |
|--------------------|-------|-----------------|
| 231-791-2          | Water | 7732-18-5       |

#### Notified classification and labelling according to CLP criteria

| Classification                    |                          | Labelling                |                                        |                                 | Specific Concentration limits, M-F | Corrosion<br>? | Exclamation mark<br>? | Affected by impurities / Additives<br>? | Additional Notified Information<br>? | Number of Notifiers<br>? | Joint Entries<br>?           |
|-----------------------------------|--------------------------|--------------------------|----------------------------------------|---------------------------------|------------------------------------|----------------|-----------------------|-----------------------------------------|--------------------------------------|--------------------------|------------------------------|
| Hazard Class and Category Code(s) | Hazard Statement Code(s) | Hazard Statement Code(s) | Supplementary Hazard Statement Code(s) | Pictograms, Signal Word Code(s) |                                    |                |                       |                                         |                                      |                          |                              |
| Not Classified                    |                          |                          |                                        |                                 |                                    |                |                       |                                         |                                      | 1157                     |                              |
|                                   |                          | H302                     |                                        | GHS05<br>GHS07<br>Dgr           |                                    |                |                       |                                         |                                      | 2                        | <a href="#">View details</a> |
|                                   |                          | H318                     |                                        |                                 |                                    |                |                       |                                         |                                      | 1                        | <a href="#">View details</a> |
|                                   |                          | NA                       |                                        |                                 |                                    |                |                       |                                         |                                      | 1                        | <a href="#">View details</a> |
| Flam. Liq. 3                      | H226                     | H226                     |                                        | GHS02<br>Wng                    |                                    |                |                       |                                         | State/Form<br>IUPAC Names            | 1                        | <a href="#">View details</a> |
| Not Classified                    |                          |                          |                                        |                                 |                                    |                |                       |                                         |                                      | 1                        |                              |
|                                   |                          | H314                     |                                        | GHS05<br>Dgr                    |                                    |                |                       |                                         | State/Form                           | 1                        | <a href="#">View details</a> |
| Acute Tox. 3                      | H301                     | H301                     |                                        |                                 |                                    |                |                       |                                         |                                      |                          |                              |

# LCSS Updates – GHS “not classified”

## Browse UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS) Tree

|                                                                                     |       |   |         |
|-------------------------------------------------------------------------------------|-------|---|---------|
| ▼ GHS Classification Tree                                                           | ?     | ↗ | 123,163 |
| ▼ Hazard Classes                                                                    | ?     |   | 122,095 |
| ▶ Environmental Hazard                                                              |       |   | 27,429  |
| ▶ Health Hazards                                                                    |       |   | 113,839 |
| ▶ Physical Hazards                                                                  |       |   | 9,417   |
| ▼ Hazard Pictograms                                                                 | ?     |   | 119,406 |
|    | GHS01 |   | 188     |
|   | GHS02 |   | 7,555   |
|  | GHS03 |   | 430     |
|  | GHS04 |   | 277     |
|  | GHS05 |   | 18,052  |

# LCSS Data access and retrieving

- Web pages – URL or scan QR code
- Pug\_view to get data blob
- For data under specific heading, using pug\_view + heading
- FTP

# LCSS Data access and retrieving

- Web pages – URL or scan QR code
  - ✓ URL: search engine, or direct URL
  - ✓ QR code generator:

[https://pubchem.ncbi.nlm.nih.gov/rest/pug\\_view/qc/long/compound/acetone/LCSS/SVG](https://pubchem.ncbi.nlm.nih.gov/rest/pug_view/qc/long/compound/acetone/LCSS/SVG)



# LCSS Data access and retrieving

- Programmatic users: Pug\_view to get data blob

- ✓ Get all page data for a given compound:

- [https://pubchem.ncbi.nlm.nih.gov/rest/pug\\_view/data/compound/180/JSON/?response\\_type=display](https://pubchem.ncbi.nlm.nih.gov/rest/pug_view/data/compound/180/JSON/?response_type=display)

- ✓ Get partial page data for specific headings:

- [https://pubchem.ncbi.nlm.nih.gov/rest/pug\\_view/data/compound/180/JSON/?response\\_type=display&heading=GHS%20Classification](https://pubchem.ncbi.nlm.nih.gov/rest/pug_view/data/compound/180/JSON/?response_type=display&heading=GHS%20Classification)

# LCSS Data – programmatic access

```
{
 "Record": {
 "RecordType": "CID",
 "RecordNumber": 180,
 "RecordTitle": "Acetone",
 "Section": [
 {
 "TOCHeading": "Structures",
 "Description": "Structure depictions and information for 2D, 3D, and

 "Section": [
 {
 "TOCHeading": "2D Structure",
 "Description": "A two-dimensional representation of the compound",
 "DisplayControls": {
 "MoveToTop": true
 },
 "Information": [
 {
 "ReferenceNumber": 117,
 "Value": {
 "Boolean": [
 true
]
 }
 }
]
 },
 {
 "TOCHeading": "3D Conformer",
 "Description": "A three-dimensional representation of the compound

 detailed information on this conformer model is described in the PubChem3D t",
 "DisplayControls": {
 "MoveToTop": true
 },
 "Information": [
 {
 "ReferenceNumber": 117,
 "Description": "Acetone",
 "Value": {
 "Number": [
 180
]
 }
 }
]
 },
 {
 "TOCHeading": "Crystal Structures",
 "Description": "This section provides links to crystallographic

 Crystallographic Data Centre (CCDC).",
```

```
<?xml version="1.0" encoding="UTF-8"?>
<Record
 xmlns="http://pubchem.ncbi.nlm.nih.gov/pug_view"
 xmlns:xs="http://www.w3.org/2001/XMLSchema-instance"
 xs:schemaLocation="http://pubchem.ncbi.nlm.nih.gov/pug_view https://pubchem.ncbi.nlm.nih.gov/pug_view/pug_view.xsd"
 >
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 regulations for dangerous goods. The GHS hazard statements, class categories, pictograms, signal words, and the precautionary statements can be found on the PubChem

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# LCSS Data access and retrieving

- FTP: <https://ftp.ncbi.nlm.nih.gov/pubchem/Compound/Extras/>

## Index of /pubchem/Compound/Extras

| Name                                      | Last modified    | Size |
|-------------------------------------------|------------------|------|
| <a href="#">Parent Directory</a>          |                  | -    |
| <a href="#">CID-Component.gz</a>          | 2019-07-18 08:49 | 36M  |
| <a href="#">CID-Date.gz</a>               | 2019-07-18 08:49 | 242M |
| <a href="#">CID-IUPAC.gz</a>              | 2019-07-18 10:36 | 1.1G |
| <a href="#">CID-InChI-Key.gz</a>          | 2019-07-18 10:34 | 4.6G |
| <a href="#">CID-MeSH</a>                  | 2019-07-18 08:50 | 147M |
| <a href="#">CID-PMID.gz</a>               | 2019-07-18 08:42 | 3.5M |
| <a href="#">CID-Parent.gz</a>             | 2019-07-18 09:24 | 321M |
| <a href="#">CID-Patent.gz</a>             | 2019-07-18 08:55 | 409M |
| <a href="#">CID-Preferred.gz</a>          | 2019-07-18 09:08 | 2.7G |
| <a href="#">CID-SID.gz</a>                | 2019-04-16 07:46 | 12M  |
| <a href="#">CID-SMILES.gz</a>             | 2019-07-18 08:59 | 1.2G |
| <a href="#">CID-Synonym-filtered.gz</a>   | 2019-07-18 09:18 | 918M |
| <a href="#">CID-Synonym-unfiltered.gz</a> | 2019-07-18 09:29 | 937M |
| <a href="#">MeSH-Pharm</a>                | 2019-07-18 09:09 | 1.1G |
| <a href="#">README-Extras</a>             | 2019-07-18 08:42 | 398K |
|                                           | 2019-04-18 13:14 | 7.0K |

# Summary

- PubChem created the LCSS aiming to help lab researchers, hygiene officers, and students to locate the chemical safety and hazard information.
- PubChem LCSS data are integrated from many authoritative sources, and all data can be tracked back to the original source.
- LCSS information can be accessed and retrieved in multiple methods.

# Thank you ...

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