

256<sup>th</sup> ACS National Meeting, Boston, August 2018

# Chemical safety information in PubChem

Jian Zhang\*, Paul Thiessen, Asta Gindulyte, Evan Bolton



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

# Outlines ...

- What is PubChem .. an overview
- What data PubChem has ..
- Chemical safety data updates:
  - CAMEO Chemicals reactivity classification
  - Pistoia Alliance Chemical Safety Library reaction alerts
- How to access and retrieve safety data ..
- Summary



# PubChem ...

- A public chemical data repository .. A public data sharing platform to submit and share chemical data
- An open chemistry database .. Free chemical information
- A chemical information hub .. Data integrated from many sources with links to provenance
- A chemical information comparison center .. Data shopping comparison
- A chemical data index

# Data Status .. <https://pubchem.ncbi.nlm.nih.gov/>

|                    |             |
|--------------------|-------------|
| Compounds:         | 96,478,070  |
| Substances:        | 247,243,896 |
| BioAssays:         | 1,252,901   |
| Tested Compounds:  | 2,978,541   |
| Tested Substances: | 4,994,132   |
| BioActivities:     | 236,790,496 |
| Protein Targets:   | 10,854      |
| Gene Targets:      | 22,108      |
| Data submitters:   | 623         |
| Countries:         | 40          |



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

PubChem

[About](#)

[Blog](#)

[Submit](#)

[Contact](#)

PubChem presents at the American Chemical Society National Meeting in Boston (August 19-23, 2018)

[Read More >](#)

# Explore Chemistry

Quickly find chemical information from authoritative sources



Try

[aspirin](#)

[EGFR](#)

[C9H8O4](#)

[57-27-2](#)

[C1=CC=C\(C=C1\)C=O](#)

[InChI=1S/C3H6O/c1-3\(2\)4/h1-2H3](#)



Draw Structure



Upload ID List



Browse Data

96M Compounds

238M Substances

282M Bioactivities

29M Literature

3M Patents

623 Data Sources

[See More Statistics >](#)

[Explore Data Sources >](#)

National Center for Biotechnology Information

NCBI

# Data ...chemical centralized and beyond

- Structures – 2D, 3D, SMILES, InChI (key)
- Properties – MP, BP, MW, MF, solubility, flash point, vapor pressure, density, crystal, spectra, ...
- Drug and medication
- Food additives
- Agrochemicals
- Safety and hazard
- Literature
- Patents
- Pathways
- Targets
- Toxicity
- Classifications
- Bioactivity
- Use and manufacture
- Nature products
- More ....
- Links to provenance



# Where to find Chemical safety information in PubChem

- PubChem compound summary page – main web page that feed chemical information
- LCSS: Laboratory Chemical Safety Summary – Subset of chemical safety information page (Ref: *Prudent Practices in the Laboratory: Handling and Management of Chemical Hazards*)
- Classification browser – Classification tree style

# Chemical safety information summary ...

## 3 major sections (headings)

Chemical and Physical Properties

Safety and Hazards

Toxicity

### + 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 Agrochemical Information
- 10 Pharmacology and Biochemistry
- 11 Use and Manufacturing
- 12 Identification
- 13 Safety and Hazards
- 14 Toxicity
- 15 Literature
- 16 Patents
- 17 Biomolecular Interactions and Pathways
- 18 Biological Test Results
- 19 Classification
- 20 Information Sources

## 13 Safety and Hazards

### 13.1 Hazards Identification

#### 13.1.1 GHS Classification



**Signal:** Danger

#### GHS Hazard Statements

Aggregated GHS information provided for each notification. Each notification may be a

Reported as not meeting GHS hazard criteria. Please visit [ECHA C&L website](#)

Of the 52 notification(s) provided by

H302 (35.91%): Harmful if swallowed  
H315 (80.13%): Causes skin irritation  
H318 (77.52%): Causes serious eye damage  
H319 (18.59%): Causes serious eye irritation  
H372 (15.71%): Causes damage to or impairment of target organ toxicity, repeated exposure

Information may vary between notifications. Percentage value in parenthesis indicates the percentage of notifications with the hazard code. Only hazard codes with

#### Precautionary Statement Codes

P260, P264, P270, P280, P301+P312,

# Chemical safety information ...

- Chemical and Physical Properties
- Safety and Hazard
- Toxicity

## **Safety and Hazards** – 11 subheadings aligned with OSHA SDS

Hazards Identification  
Safety and Hazard Properties  
First Aid Measures  
Fire Fighting Measures  
Accidental Release Measures  
Handling and Storage  
Exposure Control and Personal Protection  
Stability and Reactivity  
Transport Information  
Regulatory Information  
Other Safety Information

# Chemical safety information in compound summary ...

## Hazards Identification

- GHS Classification
- CLP Hazard Class and Category Codes
- EPA Safer Chemical
- 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

- 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
- PEL
- PEL-TWA
- PEL-STEL
- PEL-C
- REL-TWA
- REL-STEL
- REL-C
- IDLH
- Conversion
- Threshold Limit Values

## 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



# LCSS - Laboratory Chemical Safety Summary

← → ↻ Secure | <https://pubchemdocs.ncbi.nlm.nih.gov/lcss> ☆

PubChem Docs PubChem Home / Blog / Submit / Contact

⋮ Search

🏠 About

📰 News

📄 Publications

📄 Citation Guidelines

▼ What's in PubChem?

- 📄 Data Organization
- 📄 Compounds
- 📄 Substances
- 📄 BioAssays
- 📄 Targets
- 📄 Patents
- 📄 Literature
- 📄 Knowledge panels
- 📄 Laboratory Chemical Safety Summary

📄 Data Sources

▶ Search and Analysis

📄 Submissions

What's in PubChem?

## Laboratory Chemical Safety Summary (LCSS)

See a list of all compounds with LCSS

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

# LCSS - Laboratory Chemical Safety Summary

Secure <https://www.ncbi.nlm.nih.gov/pccompound>

NCBI Resources ▾ How To ▾ Sign in to NCBI

PubChem Compound PubChem Compound ▾ Search


Limits Advanced Help

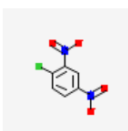
Summary ▾ 20 per page ▾ Sort by CID ▴ ▾ Send to: ▾ Filters: [Manage Filters](#)


**Links from pchierarchy**

Items: 1 to 20 of 118416

<< First < Prev Page 1 of 5921 Next > Last >>





- 

[1-Aminopropan-2-ol; 1-AMINO-2-PROPANOL; 78-96-6 ...](#)  
MW: 75.111 g/mol MF: C<sub>3</sub>H<sub>9</sub>NO  
IUPAC name: 1-aminopropan-2-ol  
Create Date: 2005-03-26  
CID: 4  
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#) [PubMed \(MeSH Keyword\)](#)
- 

[1-chloro-2,4-dinitrobenzene; 2,4-Dinitrochlorobenzene; 97-00-7 ...](#)  
MW: 202.550 g/mol MF: C<sub>6</sub>H<sub>3</sub>ClN<sub>2</sub>O<sub>4</sub>  
IUPAC name: 1-chloro-2,4-dinitrobenzene  
Create Date: 2005-03-26  
CID: 6  
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#) [PubMed \(MeSH Keyword\)](#)
- 

[1,2-dichloroethane; Ethylene dichloride; 107-06-2 ...](#)  
MW: 98.954 g/mol MF: C<sub>2</sub>H<sub>4</sub>Cl<sub>2</sub>  
IUPAC name: 1,2-dichloroethane  
Create Date: 2004-09-16

**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 (76,831)

**BioActivity Experiments**

- BioAssays, Probes (15)
- BioAssays, Active (15,890)
- BioAssays, Tested (35,700)
- Protein 3D Structures (3,106)

NCBI

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

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

PubChem OPEN  
CHEMISTRY  
DATABASE

Search Compounds



Compound Summary for CID 180

Download

Share

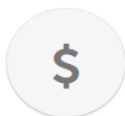
Help

# Acetone

Cite this Record



STRUCTURE



VENDORS



PHARMACOLOGY



LITERATURE



PATENTS



BIOACTIVITIES

PubChem CID: 180

Chemical Names: Acetone; 2-propanone; Propanone; 67-64-1; Dimethyl ketone; Methyl ketone [More...](#)

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

InChI Key: CSCPPACGZOO CGX-UHFFFAOYSA-N

Substance Registry: [FDA UNII](#)

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

LCSS link



Acetone is a colorless liquid us

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

from MeSH

Acetone is a colorless, volatile, flammable organic solvent. Acetone occurs naturally in plants, trees, forest fires, vehicle exhaust and as a breakdown product of animal fat metabolism. This agent may be normally present in very small quantities in urine and blood; larger amounts may be found in the urine and blood of diabetics. Acetone is toxic in high doses. (NCI04)

Pharmacology from NCI

## 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 Information Sources

etone#datasheet=lcss&section=Top

 Download

 Share

 Help



► Cite this Record

67-64-1; Dimethyl ketone; Methyl ketone

[Read about the LCSS project](#) 

### GHS Classification



**Danger**

#### Hazard Statements

Highly Flammable liquid and vapor [**Danger** Flammable liquids]

Causes serious eye irritation [**Warning** Serious eye damage/eye irritation]

May cause drowsiness or dizziness [**Warning** Specific target organ toxicity, single exposure; Narcotic effects]

#### Precautionary Statement Codes

P233, P240, P241, P242, P243, P261, P271, P280, P303+P361+P353, P304+P340, P305+P351+P338, P312, P313, P370+P378, P403+P233, P403+P235, P405, and P501

(The corresponding statement to each P-code can be found [here](#).)

► from EU REGULATION (EC) No 1272/2008, Safe Work Australia - HCIS



# Classification browser ...

The classification browser allows users to browse the distribution of PubChem data among nodes in the hierarchy of interest, thereby providing an aggregate view of PubChem data. It also allows you to search for PubChem records annotated with the desired hierarchy/term, providing a powerful way to quickly find the subset of PubChem records.

**Classification trees: major: 16. Safety info related: 4**

# Chemical Safety information from the Classification browser

- CA
- EF
- Pu
- UN

https



## PubChem Classification Browser

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

Select classification

UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS) ▾

MeSH: MeSH Tree

CAMEO Chemicals: CAMEO Chemical Reactivity Classification

ChEBI: ChEBI Ontology

ChEMBL: Target Tree

ChemIDplus: ChemIDplus Chemical Information Classification

ENZYME: Enzyme Classification

EPA Safer Choice: EPA Safer Chemical Ingredients Classification

B FDA Pharm Classes: FDA Pharmacological Classification

Gene Ontology >

IUPHAR/BPS Guide to PHARMACOLOGY: Target Classification >

KEGG >

LIPID MAPS: LIPID MAPS classification system for lipids

NCBI Taxonomy: Taxonomy

PubChem >

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

Search selected classification by

Keyword ▾

Enter desired search term

Search

for globally uniform physical, environmental, and health and safety information on  
d environmental hazards of chemical substances and mixtures and sets up

Tree

PubChem BioAssay Classification

PubChem Compound TOC

# Chemical safety information ... Updates

- Cameo Chemicals reactivity classification
- Pistoia Alliance Chemical Safety Library  
CSL's Reaction alerts information

# Update - CAMEO Chemicals Reactivity Classification

CAMEO Chemicals classify chemicals into 68 reactive categories according to structures and reactions. PubChem integrated the reactivity information and make it a special tree display for quick and convenient browsing

- Descriptions
  - Flammability
  - Reactivity
  - Toxicity
  - Others
- Reactivity Documentation

<https://pubchem.ncbi.nlm.nih.gov/classification/#hid=86>



# PubChem Classification Browser

[Help](#)

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

Select classification

CAMEO Chemicals

Search selected classification by

Keyword

Enter desired search term

Search

Classification description (from CAMEO Chemicals)

CAMEO Chemical Reactivity Classification was created based on the reactive groups. [More...](#)

Data type counts to display

None

Substance

Compound

Display zero count nodes?

Yes

No

## Browse CAMEO Chemicals Tree

- ▼ CAMEO Chemical Reactivity Classification ? ↗ 4,837
  - ▶ Acetals, Ketals, Hemiacetals, and Hemiketals ? ↗ 70
  - ▶ Acids, Carboxylic ? ↗ 203
  - ▶ Acids, Strong Non-oxidizing ? ↗ 42
  - ▶ Acids, Strong Oxidizing ? ↗ 25
  - ▶ Acids, Weak ? ↗ 95
  - ▶ Acrylates and Acrylic Acids ? ↗ 54
  - ▶ Acyl Halides, Sulfonyl Halides, and Chloroformates ? ↗ 120
  - ▶ Alcohols and Polyols ? ↗ 604
  - ▶ Aldehydes ? ↗ 75
  - ▶ Alkynes, with Acetylenic Hydrogen ? ↗ 10
  - ▶ Alkynes, with No Acetylenic Hydrogen ? ↗ 11
  - ▶ Amides and Imides ? ↗ 437

PubChem Classification Bro x PubChem Compounds from x

Secure | [https://www.ncbi.nlm.nih.gov/pccompound?DbFrom=pchierarchy&Cmd=Link&Db=pccompound&LinkName=pchierarchy\\_pccompound&IdsFromResult=3262498](https://www.ncbi.nlm.nih.gov/pccompound?DbFrom=pchierarchy&Cmd=Link&Db=pccompound&LinkName=pchierarchy_pccompound&IdsFromResult=3262498)

NCBI Resources How To Sign in to NCBI

PubChem Compound PubChem Compound Search Limits Advanced Help

Summary 20 per page Sort by Default order Send to Filters: [Manage Filters](#)

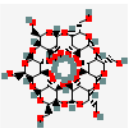
Links from pchierarchy

Items: 1 to 20 of 604

<< First < Prev Page 1 of 31 Next > Last >>

☐

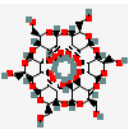
1.



[10016-20-3](#)  
MW: 972.846 g/mol MF: C<sub>38</sub>H<sub>80</sub>O<sub>30</sub>  
Create Date: 2018-07-31  
CID: 134691989  
[Summary](#) [Similar Compounds](#) [Same Parent Connectivity](#)

☐

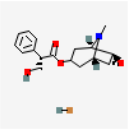
2.



[a-cyclodextrin: 10016-20-3](#)  
MW: 972.846 g/mol MF: C<sub>38</sub>H<sub>80</sub>O<sub>30</sub>  
Create Date: 2018-07-21  
CID: 134690639  
[Summary](#) [Similar Compounds](#) [Same Parent Connectivity](#)

☐

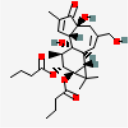
3.



[Atroscine Hydrobromide: 114-49-8](#)  
MW: 384.270 g/mol MF: C<sub>17</sub>H<sub>22</sub>BrNO<sub>4</sub>  
Create Date: 2018-07-17  
CID: 134688931  
[Summary](#) [Similar Compounds](#) [Same Parent Connectivity](#) [Mixture/Component Compounds](#)


☐

4.




[Phorbol-12,13-dibutyrate](#)  
MW: 504.620 g/mol MF: C<sub>28</sub>H<sub>40</sub>O<sub>8</sub>  
Create Date: 2018-07-17  
CID: 134688659  
[Summary](#) [Similar Compounds](#) [Same Parent Connectivity](#) [PubMed \(MeSH Keyword\)](#)


☐





[mezerein: 34807-41-5](#)

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 (305)

**BioActivity Experiments**  
BioAssays, Active (266)  
BioAssays, Tested (385)  
Protein 3D Structures (99)  
Structure Of A Protease 2 (8)  
Improved Crystal Structure Of Pseudomonas Aeruginosa Occk1 (Opdk) (8)  
Structure Of A Protease 1 (8)  
... All 12,372 Structures

**BioMedical Annotation**  
Pharmacological Actions (271)  
Anti-Bacterial Agents (33)  
Antineoplastic Agents, Phytogenic (26)  
Tubulin Modulators (17)  
... All 110 Pharmacological Actions

Alcohols and Polyols | CAMEO

Secure | https://cameochemicals.noaa.gov/react/4

Home

Help

Search Chemicals

New Search

Search Results

MyChemicals

chemicals: 0

View MyChemicals

Predict Reactivity

Mobile Site

Download on the App Store

GET IT ON Google Play

CAMEO Chemicals

Reactive Group Datasheet

Alcohols and Polyols

What are reactive groups?

Description

Flammability

Reactivity

Toxicity

Other Characteristics

Examples

Reactivity Documentation

Add to MyChemicals

Print Friendly Page

Reactive groups are categories of chemicals that typically react in similar ways because they are similar in their chemical structure. Each substance with a chemical datasheet has been assigned to one or more reactive groups, and CAMEO Chemicals uses the reactive group assignments to make its reactivity predictions. [More info about reactivity predictions...](#)

If you can't find a chemical in the database--but you know what reactive group it belongs in--you can add the reactive group to MyChemicals instead in order to see the reactivity predictions.

There are [411 chemical datasheets](#) assigned to this reactive group.

Many alcohols are highly flammable (with flash points below 100 degrees F). Especially dangerous are methanol and ethyl alcohol, because of their wide flammability limits. Polyols are generally combustible. Their generally low volatility means that they are poorly flammable.

Flammable and/or toxic gases are generated by the combination of these materials with alkali metals, nitrides, and strong reducing agents. They react with anhydrides to form acids and esters, generating noticeable heat, and also with oxoacids and carboxylic acids to form esters plus water, but the heat of reaction in the latter case typically is low. Oxidizing agents convert them to aldehydes or ketones. They exhibit both weak acid and weak base behavior. They may initiate the polymerization of isocyanates and epoxides.

Alcohols and polyols vary widely in toxicity. Among the most toxic are methyl and allyl alcohol, which act as nervous system depressants.

These materials are organic compounds containing one or more hydroxyl (-OH) groups linked to hydrocarbon groups. Alcohols may have straight-chain, branched-chain or ring structures. Polyols contain two or more hydroxyl groups; diols contain exactly two hydroxyl groups, each attached to a different carbon atom.

Ethyl alcohol, methanol, propanol, butanol, ethylene glycol, hexanol, allyl alcohol, amyl alcohol, benzyl alcohol, cyclopentanol, glycerol, isopropyl alcohol, isobutyl alcohol.

PubChem Classification Browser

Secure | <https://pubchem.ncbi.nlm.nih.gov/classification/#hid=86>

▶ Acrylates and Acrylic Acids ? ↗ 54

▶ Acyl Halides, Sulfonyl Halides, and Chloroformates ?

▼ Alcohols and Polyols ? ↗ 54

▼ Flammability

▼ Other Characteristics

▼ Reactivity Documentation

Many alcohols are highly flammable (with flash points below 100 degrees F). Especially dangerous are methanol and ethyl alcohol, because of their wide flammability limits. Polyols are generally combustible. Their generally low volatility means that they are poorly flammable.

Many alcohols are highly flammable (with flash points below 100 degrees F). Especially dangerous are methanol and ethyl alcohol, because of their wide flammability limits. Polyols are generally combustible. Their generally low volatility means that they are poorly flammable.

These materials are organic compounds containing one or more hydroxyl (-OH) groups linked to hydrocarbon groups. Alcohols may have straight-chain, branched-chain, or ring structures. Polyols contain two or more hydroxyl groups; diols contain exactly two hydroxyl groups, each attached to a different carbon atom.

Flammable and/or toxic gases are generated by the combination of these materials with alkali metals, nitrides, and strong reducing agents. They react with anhydrides to form acids and esters, generating noticeable heat.... click [?] to see more. ?

▶ Aldehydes ? ↗ 75

▶ Alkynes, with Acetylenic Hydrogen ? ↗ 10

▶ Alkynes, with No Acetylenic Hydrogen ? ↗ 11

Alcohols and Polyols | CAMEO Chemicals

Secure | <https://cameochemicals.noaa.gov/react/4>

Home

Help

Search Chemicals

New Search

Search Results

MyChemicals

chemicals: 0

View MyChemicals

Predict Reactivity

Mobile Site

Download on the App Store

GET IT ON Google Play

Reactive Group Datasheet

Add to MyChemicals

Print Friendly Page

Alcohols and Polyols

What are reactive groups?

Reactive groups are categories of chemicals that typically react in similar ways because they are similar in their chemical structure. Each substance with a chemical datasheet has been assigned to one or more reactive groups, and CAMEO Chemicals uses the reactive group assignments to make its reactivity predictions. [More info about reactivity predictions...](#)

If you can't find a chemical in the database--but you know what reactive group it belongs in--you can add the reactive group to MyChemicals instead in order to see the reactivity predictions.

There are [411 chemical datasheets](#) assigned to this reactive group.

Description

Flammability

Many alcohols are highly flammable (with flash points below 100 degrees F). Especially dangerous are methanol and ethyl alcohol, because of their wide flammability limits. Polyols are generally combustible. Their generally low volatility means that they are poorly flammable.

Reactivity

Flammable and/or toxic gases are generated by the combination of these materials with alkali metals, nitrides, and strong reducing agents. They react with anhydrides to form acids and esters, generating noticeable heat, and also with oxoacids and carboxylic acids to form esters plus water, but the heat of reaction in the latter case typically is low. Oxidizing agents convert them to aldehydes or ketones. They exhibit both weak acid and weak base behavior. They may initiate the polymerization of isocyanates and epoxides.

Toxicity

Alcohols and polyols vary widely in toxicity. Among the most toxic are methyl and allyl alcohol, which act as nervous system depressants.

Other Characteristics

These materials are organic compounds containing one or more hydroxyl (-OH) groups linked to hydrocarbon groups. Alcohols may have straight-chain, branched-chain or ring structures. Polyols contain two or more hydroxyl groups; diols contain exactly two hydroxyl groups, each attached to a different carbon atom.

Examples

Ethyl alcohol, methanol, propanol, butanol, ethylene glycol, hexanol, allyl alcohol, amyl alcohol, benzyl alcohol, cyclopentanol, glycerol, isopropyl alcohol, isobutyl alcohol.

Reactivity Documentation

# CAMEO Chemicals Reactivity Classification

- Reactivity Documentation
  - Reactivity summary when one reactive group (chemical) mixed with another one.

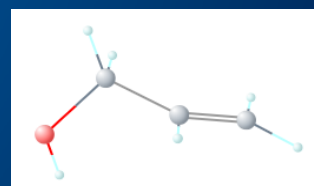
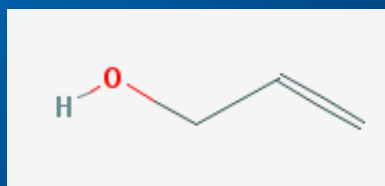
PubChem Classification Bro x

Secure | <https://pubchem.ncbi.nlm.nih.gov/classification/#hid=86>

- ▶ Acyl Halides, Sulfonyl Halides, and Chloroformates ? ↗ 120
- ▼ Alcohols and Polyols ? ↗ 604
  - ▶ Reactivity summary when Alcohols and Polyols mixed with Acids, Strong Oxidizing:
    - ▶ Explosive: Reaction products may be explosive or sensitive to shock or friction
    - ▶ Flammable: Reaction products may be flammable
    - ▶ Generates gas: Reaction liberates gaseous products and may cause pressurization
    - ▶ Intense or explosive reaction: Reaction may be particularly intense, violent, or explosive
    - ▶ Toxic: Reaction products may be toxic
    - ▶ May produce the following gases:
      - Aldehydes
      - Chlorine Dioxide
      - Hydrocarbons
      - Nitrogen Oxides
      - Halogen Oxides
- ▶ Acids, Weak ? ↗
- ▶ Acrylates and Acrylic Acids ? ↗
- ▶ Acyl Halides, Sulfonyl Halides, and Chloroformates ? ↗

# Case study: an individual compound vs classification tree

- Example: allyl alcohol
- CID 7858



Space replacement: + or %20 or \_

<https://pubchem.ncbi.nlm.nih.gov/compound/allyl+alcohol>

PubChem base URL

Database

compound

PubChem Classification Browser

Secure | <https://pubchem.ncbi.nlm.nih.gov/classification/#hid=86&cid=7858&view=list>

Select classification: CAMEO Chemicals

Search selected classification by: [Search] [Clear]

Data type counts: [None] [Substances]

Showing tree for node: "Alcohols and Polyols"

- ▼ CAMEO Chemical Reactivity Classification [?] [↗] 4,837
  - ▼ Alcohols and Polyols [?] [↗] 604
    - ▶ Flammability
    - ▶ Other Characteristics
    - ▶ Reactivity
    - ▼ Reactivity Documentation (when Alcohols and Polyols mixed with other chemical agents)
      - ▶ Acetals, Ketals, Hemiacetals, and Hemiketals [?] [↗]
      - ▶ Acids, Carboxylic [?] [↗]
      - ▶ Acids, Strong Non-oxidizing [?] [↗]
      - ▶ Acids, Strong Oxidizing [?] [↗]
      - ▶ Acids, Weak [?] [↗]
      - ▶ Acrylates and Acrylic Acids [?] [↗]
      - ▶ Acyl Halides, Sulfonyl Halides, and Chloroformates [?] [↗]
      - ▶ Alcohols and Polyols [?] [↗]
      - ▶ Aldehydes [?] [↗]
      - ▶ Alkynes, with Acetylenic Hydrogen [?] [↗]
      - ▶ Alkynes, with No Acetylenic Hydrogen [?] [↗]
      - ▶ Amides and Imides [?] [↗]
      - ▶ Amines, Aromatic [?] [↗]

CAMEO Chemicals

Results 1 to 3 of 3

1. Alcohols and Polyols  
Reactive group: [?] [↗]  
Class: [?] [↗]  
CA: [?]
2. Hydrocarbons  
Reactive group: [?] [↗]  
Class: [?] [↗]  
CA: [?]
3. Polymerization  
Reactive group: [?] [↗]  
Class: [?] [↗]  
CA: [?]



PubChem Classification Browser

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

Select classification: CAMEO Chemicals

Search selected classification by: CID 7858

Search: Search Clear

Classification description (from CAMEO Chemicals): CAMEO Chemical Reactivity Classification was created by the U.S. Environmental Protection Agency (EPA) to provide a systematic way of classifying chemicals based on their reactivity. More...

Data type counts to display: None Substance Compound

View type: Tree List

Page size: 10 20 50 100 200

Filter by Entrez History: Choose one

CAMEO Chemicals Search for CID 7858

Results 1 to 3 of 3

1. Alcohols and Polyols [604](#)  
Reactive group: Alcohols and Polyols  
**Classification:**  
CAMEO Chemical Reactivity Classification > Alcohols and Polyols
2. Hydrocarbons, Aliphatic Unsaturated [625](#)  
Reactive group: Hydrocarbons, Aliphatic Unsaturated  
**Classification:**  
CAMEO Chemical Reactivity Classification > Hydrocarbons, Aliphatic Unsaturated
3. Polymerizable Compounds [208](#)  
Reactive group: Polymerizable Compounds  
**Classification:**  
CAMEO Chemical Reactivity Classification > Polymerizable Compounds

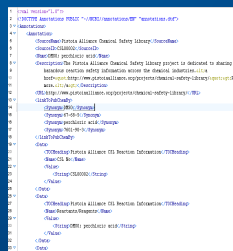
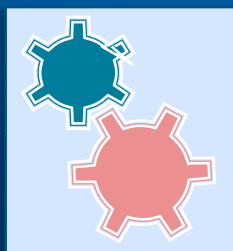
javascript:void(0);

A quick search will give the same result

# Update: the reaction alerts from Pistoia Alliance CSL

Reactivity information when one chemical meet another one.

| COL No  | Reaction Class | Reaction Type | COL No  | INCHI    | INCHI KEY | SMILES   |
|---------|----------------|---------------|---------|----------|-----------|----------|
| C000001 | ACID           | Permeant      | C000001 | ACID     | Permeant  | ACID     |
| C000002 | Alkaline       | Permeant      | C000002 | Alkaline | Permeant  | Alkaline |
| C000003 | Alkaline       | Permeant      | C000003 | Alkaline | Permeant  | Alkaline |
| C000004 | Alkaline       | Permeant      | C000004 | Alkaline | Permeant  | Alkaline |
| C000005 | Alkaline       | Permeant      | C000005 | Alkaline | Permeant  | Alkaline |
| C000006 | Alkaline       | Permeant      | C000006 | Alkaline | Permeant  | Alkaline |
| C000007 | Alkaline       | Permeant      | C000007 | Alkaline | Permeant  | Alkaline |
| C000008 | Alkaline       | Permeant      | C000008 | Alkaline | Permeant  | Alkaline |
| C000009 | Alkaline       | Permeant      | C000009 | Alkaline | Permeant  | Alkaline |
| C000010 | Alkaline       | Permeant      | C000010 | Alkaline | Permeant  | Alkaline |



| Pistoia Alliance CSL Reactivity Alerts  |  |
|---|--|
| Pistoia Alliance CSL Reactivity Alerts: 1 of 13 (Pistoia Alliance CSL Reaction Information)   |  |
| CSL No  | CSL00007                               |
| Reactants/Reagents  | CARBON DIOXIDE, SODIUM AZIDE           |
| CSG Category  | Explosive                              |
| Warning Message   | Potentially explosive                  |
| Source Reference  | User Reported                          |
| CSL Status  | Approved                               |
| Modified Date   | 2/27/2018                              |
| * from Pistoia Alliance Chemical Safety Library   |  |
| Source: Pistoia Alliance Chemical Safety Library<br>Reagent Name: CARBON DIOXIDE, SODIUM AZIDE<br>URL: <a href="https://www.pistoiaalliance.org/chemical-safety-library/">https://www.pistoiaalliance.org/chemical-safety-library/</a><br>Description: The Pistoia Alliance Chemical Safety Library project is dedicated to sharing laboratory reaction safety information across the chemical industries. Read more. |  |
| Pistoia Alliance CSL Reactivity Alerts: 2 of 13 (Pistoia Alliance CSL Reaction Information)   |  |
| CSL No  | CSL00078                               |
| Reactants/Reagents  | SODIUM AZIDE, PHOSPHORUS PENTACHLORIDE |
| CSG Category  | Explosive                              |
| Warning Message   | Highly explosive                       |
| Source Reference  | User Reported                          |
| CSL Status  | Approved                               |
| Modified Date   | 2/27/2018                              |

Select classification Search selected classification by

Classification description (from PubChem)

This classification was created automatically from the PubChem Compound TOC on 2018/07/31.

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: Cor  
Removed Synonyms, Create Date, Modify Date, Record Title, Related Compounds, Re

Data type counts to display    Display zero count nodes?    Filter by Entrez History

**None**    **Compound**    **Yes**    No    Choose one

[Browse PubChem: PubChem Compound TOC Tree](#)

- PubChem Compound TOC ? 31,354,895
- ▶ Agrochemical Information ? 1,986
  - ▶ Biologic Description ? 522,034
  - ▶ Biological Test Results ? 2,975,229
  - ▶ Biomolecular Interactions and Pathways ? 56,078
  - ▶ Chemical and Physical Properties ? 731,742
  - ▶ Classification ? 17,577,635
  - ▶ Drug and Medication Information ? 13,233
  - ▶ Element Information ?
  - ▶ Food Additives and Ingredients ? 6,885
  - ▶ Identification ? 5,734
  - ▶ Information Sources ? 19,003,971
  - ▶ Literature ? 1,031,003
  - ▶ Names and Identifiers ? 1,285,178
  - ▶ Patents ? 21,211,974
  - ▶ Pharmacology and Biochemistry ? 122,424
  - ▶ Related Records ? 5,166,044
  - ▶ Safety and Hazards ? 121,086
  - ▶ Toxicity ? 11,243
  - ▶ Use and Manufacturing ? 15,432
- 3D Status ? 5,761,938
- LCSS ? 118,387

- The screenshot displays the search results for 'Pistoia Alliance' in the NIOSH Chemical Hazards Database. The results are organized into a hierarchical tree structure. The top-level categories are 'Identification' (5,734 records) and 'Information Sources' (19,003,971 records). Under 'Information Sources', the 'Burnham Center for Chemical Genomics' is listed with 57,854 records, and 'CAMEO Chemicals' is listed with 4,929 records. The 'Related Records' section shows 5,166,044 records. The 'Safety and Hazards' section is expanded, showing various categories with their respective record counts: 'Accidental Release Measures' (8,409), 'Exposure Control and Personal Protection' (7,179), 'Fire Fighting Measures' (6,409), 'First Aid Measures' (5,197), 'Handling and Storage' (7,307), 'Hazards Identification' (119,691), 'Other Safety Information' (1,850), 'Regulatory Information' (5,423), 'Safety and Hazard Properties' (2,990), and 'Stability and Reactivity' (5,978). Under 'Stability and Reactivity', the 'Reactivity Alerts' category is expanded, showing 'Pistoia Alliance CSL Reactivity Alerts' (150 records), 'Air and Water Reactions' (4,743), 'Reactive Group' (4,743), 'Reactivities and Incompatibilities' (2,866), and 'Reactivity Profile' (4,544). The 'Pistoia Alliance CSL Reactivity Alerts' entry is highlighted in yellow.

| Category                                 | Record Count |
|--|--------------|
| Identification                           | 5,734        |
| Information Sources                      | 19,003,971   |
| Burnham Center for Chemical Genomics     | 57,854       |
| CAMEO Chemicals                          | 4,929        |
| Related Records                          | 5,166,044    |
| Safety and Hazards                       | 21,086       |
| Accidental Release Measures              | 8,409        |
| Exposure Control and Personal Protection | 7,179        |
| Fire Fighting Measures                   | 6,409        |
| First Aid Measures                       | 5,197        |
| Handling and Storage                     | 7,307        |
| Hazards Identification                   | 119,691      |
| Other Safety Information                 | 1,850        |
| Regulatory Information                   | 5,423        |
| Safety and Hazard Properties             | 2,990        |
| Stability and Reactivity                 | 5,978        |
| Reactivity Alerts                        | 1,693        |
| Pistoia Alliance CSL Reactivity Alerts   | 150          |
| Air and Water Reactions                  | 4,743        |
| Reactive Group                           | 4,743        |
| Reactivities and Incompatibilities       | 2,866        |
| Reactivity Profile                       | 4,544        |

Acetone | CH<sub>3</sub>-CO-CH<sub>3</sub> - PubChem

Secure

https://pubchem.ncbi.nlm.nih.gov/compound/180#section=Pistoia-Alliance-CSL-Reactivity-Alerts

Acetone

Download

Share

Help

Contents

1 2D Structure

2 3D Conformer

3 Names and Identifiers

4 Chemical and Physical Properties

5 Related Records

6 Chemical Vendors

7 Food Additives and Ingredients

8 Agrochemical Information

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

12.8.3.1 Pistoia Alliance CSL Reactivity Alerts

Pistoia Alliance CSL Reactivity Alerts: 1 of 7 (Pistoia Alliance CSL Reaction Information)

|                    |   |
|--------------------|---|
| CSL No             | CSL00003                                      |
| Reactants/Reagents | ACETONE; <a href="#">sodium percarbonate</a>  |
| 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

Source: [Pistoia Alliance Chemical Safety Library](#)

Record Name: ACETONE; sodium percarbonate

URL: <http://www.pistoiaalliance.org/projects/chemical-safety-library/>

Description: The Pistoia Alliance Chemical Safety Library project is dedicated to sharing hazardous reaction safety information across the chemical industries.[Read more.](#)

Pistoia Alliance CSL Reactivity Alerts: 2 of 7 (Pistoia Alliance CSL Reaction Information)

|                    |  |
|--------------------|--|
| CSL No             | CSL00009                                   |
| Reactants/Reagents | ACETONE; <a href="#">Hydrogen peroxide</a> |
| GHS Category       | Explosive                                  |

# Data Retrieving ...

- Web page direct
- Using classification browser
- Using the sources page
- Using pug-view services – programmatic access

# Data retrieving .. Sources page

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

https://pubchem.ncbi.nlm.nih.gov/rest/pug\_view/annotations/heading/JSON/?source=Pistoia%20Alliance%20Chemical%20Safety%20Library&heading=Pistoia...

```
{
  "Annotations": {
    "Annotation": [
      {
        "SourceName": "Pistoia Alliance Chemical Safety Library",
        "SourceID": "CSL00002",
        "Name": "DMSO; perchloric acid",
        "Description": "The Pistoia Alliance Chemical Safety Library project is dedicated to sharing hazardous reaction safety information across the chemical industries.<a href='\"http://www.pistoiaalliance.org/projects/chemical-safety-library/\"'>Read more.</a>",
        "URL": "http://www.pistoiaalliance.org/projects/chemical-safety-library/",
        "LinkToPubChemBy": {
        },
        "Data": [
          {
            "TOCHeading": "Pistoia Alliance CSL Reaction Information",
            "Name": "CSL No",
            "Value": {
              "String": [
                "CSL00002"
              ]
            }
          },
          {
            "TOCHeading": "Pistoia Alliance CSL Reaction Information",
            "Name": "Reactants/Reagents",
            "Value": {
              "String": [
                "DMSO; perchloric acid"
              ]
            }
          },
          {
            "TOCHeading": "Pistoia Alliance CSL Reaction Information",
            "Name": "Reaction Class",
            "Value": {
              "String": [
                "oxidation"
              ]
            }
          },
          {
            "TOCHeading": "Pistoia Alliance CSL Reaction Information",
```

# Data retrieving .. Pug\_view APIs

PubChem Pug\_view URL for Pistoia Alliance CSL data on acetone compound summary:

```
https://pubchem.ncbi.nlm.nih.gov/rest/pug_view/data/compound/180/JSON/?heading=Pistoia+Alliance+CSL+Reactivity+Alerts
```

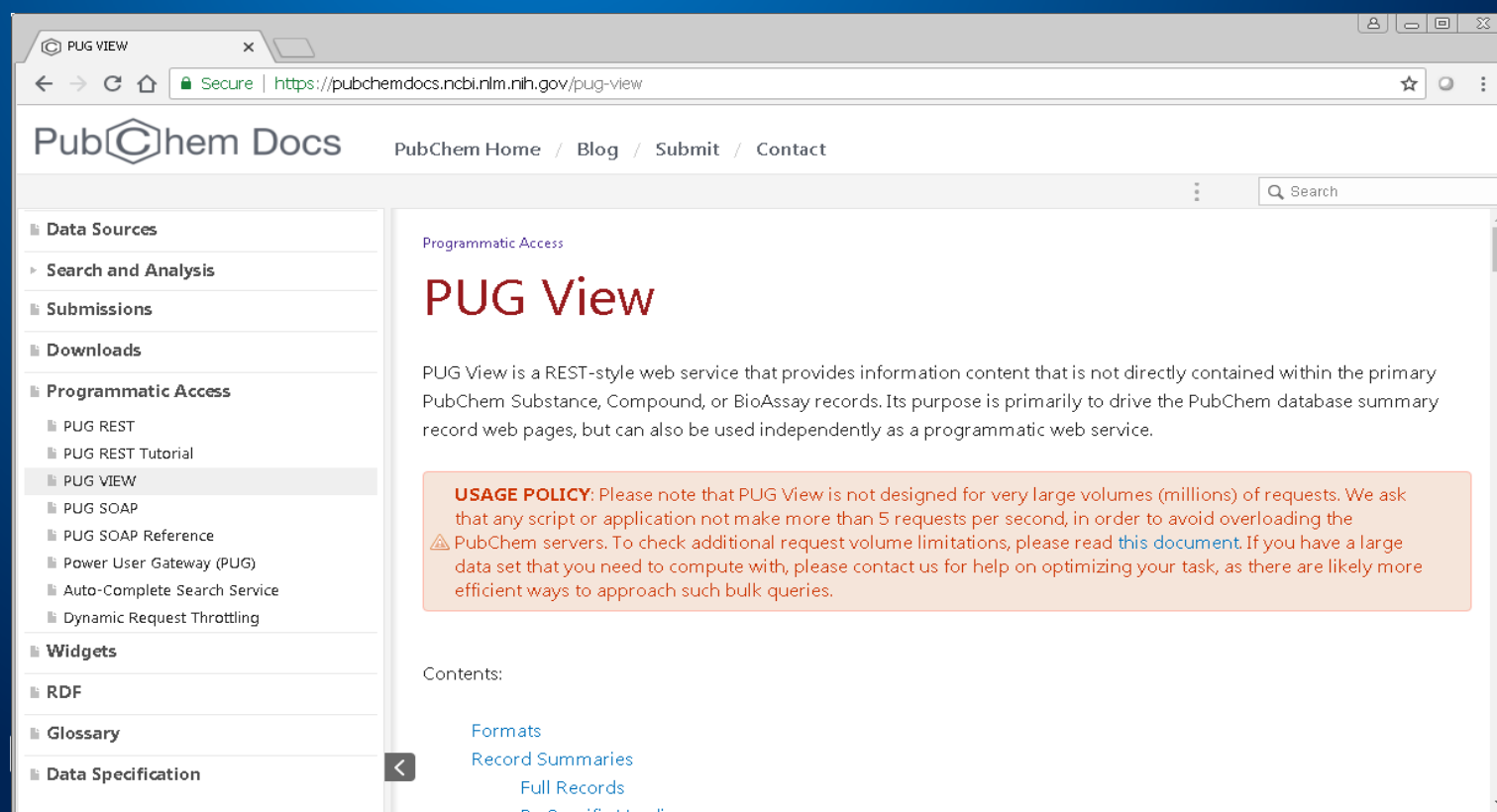


https://pubchem.ncbi.nlm.nih.gov/rest/pug\_view/data/compound/180/JSON/?heading=Pistoia+Alliance+CSL+Reactivity+Alerts

```
{
  "Record": {
    "RecordType": "CID",
    "RecordNumber": 180,
    "Section": [
      {
        "TOCHeading": "Safety and Hazards",
        "Description": "Safety and hazards information, properties, management techniques, reactivities and incompatibilities, first aid treatments, and more.",
        "Section": [
          {
            "TOCHeading": "Stability and Reactivity",
            "Description": "Stability and reactivity lists chemical stability and possibility of hazardous reactions. (See also Stability section under the Experimental Properties if available)",
            "Section": [
              {
                "TOCHeading": "Reactivity Alerts",
                "Description": "Special alerts if the chemical is especially reactive",
                "Information": [
                  {
                    "ReferenceNumber": 1,
                    "Name": "Reactivity Alerts",
                    "StringValue": "Highly Flammable<br>"
                  }
                ]
              },
              {
                "TOCHeading": "Pistoia Alliance CSL Reactivity Alerts",
                "Description": "Chemical reaction alert information from the Pistoia Alliance Chemical Safety Library",
                "HintGroupSubsectionsByReference": true,
                "Section": [
                  {
                    "TOCHeading": "Pistoia Alliance CSL Reaction Information",
                    "Description": "Chemical reaction information from the Pistoia Alliance Chemical Safety Library",
                    "Information": [
                      {
                        "ReferenceNumber": 40,
                        "Name": "CSL No",
                        "StringValue": "CSL00003"
                      },
                      {
                        "ReferenceNumber": 40,
                        "Name": "Reactants/Reagents",

```

# Data retrieving .. Pug\_view APIs



The screenshot shows a web browser window displaying the PubChem Docs PUG View page. The browser's address bar shows the URL <https://pubchemdocs.ncbi.nlm.nih.gov/pug-view>. The page header includes the PubChem Docs logo and navigation links: PubChem Home / Blog / Submit / Contact. A search bar is located in the top right corner.

The left sidebar contains a navigation menu with the following sections:

- Data Sources
- Search and Analysis
- Submissions
- Downloads
- Programmatic Access
  - PUG REST
  - PUG REST Tutorial
  - PUG VIEW**
  - PUG SOAP
  - PUG SOAP Reference
  - Power User Gateway (PUG)
  - Auto-Complete Search Service
  - Dynamic Request Throttling
- Widgets
- RDF
- Glossary
- Data Specification

The main content area is titled "PUG View" under the "Programmatic Access" section. It describes PUG View as a REST-style web service that provides information content not directly contained within the primary PubChem Substance, Compound, or BioAssay records. Its purpose is primarily to drive the PubChem database summary record web pages, but it can also be used independently as a programmatic web service.

A **USAGE POLICY** box states: "Please note that PUG View is not designed for very large volumes (millions) of requests. We ask that any script or application not make more than 5 requests per second, in order to avoid overloading the PubChem servers. To check additional request volume limitations, please read [this document](#). If you have a large data set that you need to compute with, please contact us for help on optimizing your task, as there are likely more efficient ways to approach such bulk queries."

Below the description, a "Contents:" section lists the following links:

- Formats
- Record Summaries
- Full Records
- Power User Gateway

The NCBI logo is visible in the bottom right corner of the page.

# Summary

- PubChem provides various chemical safety information as well as the link backs to original data sources.
- CAMEO Chemicals classification allows users find warning message and/or reaction activity potentials.
- Pistoia Alliance CSL's reactivity data is helpful for chemist especially the junior chemistry student when handle chemical reagents.
- The chemical data in PubChem can be retrieved in individual or batch compounds, with browsing or programmatical way.

# Thanks you ...



Evan Bolton      Tiejun Cheng  
Asta Gindulyte   Jane He  
Ben Shoemaker   Sunghwan Kim  
Paul Thiessen      Leon Li  
Siqian He          Leonid Zaslavsky  
Bo Yu  
Jie Chen

This research was supported by the Intramural Research Program of the NIH, National Library of Medicine.



Carmen Nitsche  
Gabrielle Whittick  
Mark Manfredi  
Leah Rae McEwen  
Ralph Stuart