

Data, data everywhere, nor any bit processable
Opportunities for amalgamating and opening up
chemical data and information relevant to hazard
recognition and safety planning

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Leah McEwen 2

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1 U.S. National Center for Biotechnology Information (NCBI)

2 Clark Library, Cornell University



ease note ...

am a chemist

am an informatician

work with data .lots. of it

help to create public interfaces to chemical (biology) information

work with health and safety professionals, authoritative sources of H&S information, (increasingly) those involved in H&S communities (including chemistry librarians

am not a chemical health and safety (H&S) professional



Special thanks

Chemical Health and Safety collaborators

- Especially: Leah McEwen, Ye Li, Ralph Stuart

Software collaborators

- Especially: Daniel Lowe and Roger Sayle (NextMove Software .. LeadMine)

All Contributors and Collaborators

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



PubChem resource

Primary aim is to provide information known about chemical substances

- Contains authoritative resources
- Contains manually curated resources
- Includes health and safety
- There are errors
 - Authoritative doesn't mean error free
 - Curated doesn't mean error free
- We DO NOT curate (known errors reported , filtered)
- We can leverage curated content

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

The screenshot shows the PubChem website homepage. At the top, there is a navigation bar with links for 'Databases', 'Upload', 'Services', 'Help', and 'more'. A 'Today's Statistics' dropdown menu is open, displaying the following data:

Compounds:	60,773,408
Substances:	157,310,902
BioAssays:	1,154,357
Tested Compounds:	2,090,746
Tested Substances:	3,170,077
RNAi BioAssays:	65
BioActivities:	229,468,647
Protein Targets:	9,952
Gene Targets:	57,041

Below the statistics, there is a search bar with buttons for 'BioAssay' and 'Compound'. A message box states: 'New The Laboratory Chemical Safety Summary (LCSS) view is now available in PubChem. Read more...'. At the bottom, there are links for 'Write to Helpdesk', 'Disclaimer', 'Privacy Statement', 'Accessibility', and 'Data Citation Guidelines', along with the text 'National Center for Biotechnology Information NLM | NIH | HHS'.

NATIONAL
L



NATIONAL FIRE PROTECTION ASSOCIATION
The leading information and knowledge resource on fire, electrical and related hazards



ChemIDplus: A TOXNET DA

Chemical Health and Safety Data Sources



Biological Safety Data Sheets

NIOSH Pocket Guide to Chemical Hazards



http://

Does each organization (or scientist) use their own favorite data source(s)?



Department



National Chemical Sa

Do these various data sources provide consistent information (gaps, errors)?

SIRI MSDS Index

Environmental Hea

cer



SDS and Chemi

How does the health and safety decision change with different information (or lack of it)?



Substance Fact S



TOXNET DATABASE

INDEX FREE on the

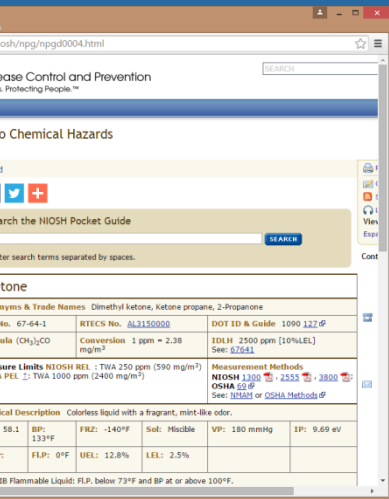


U.S. DEPARTMENT OF JUSTICE ★ DRUG ENFORCEMENT ADMINISTRATION
OFFICE OF DIVERSION CONTROL

U.S. National Library of Medicine



Chemical Health and Safety Information



OSHA Occupational Safety and Health Administration

Search the NIOSH Pocket Guide

Enter search terms separated by spaces.

Acetone

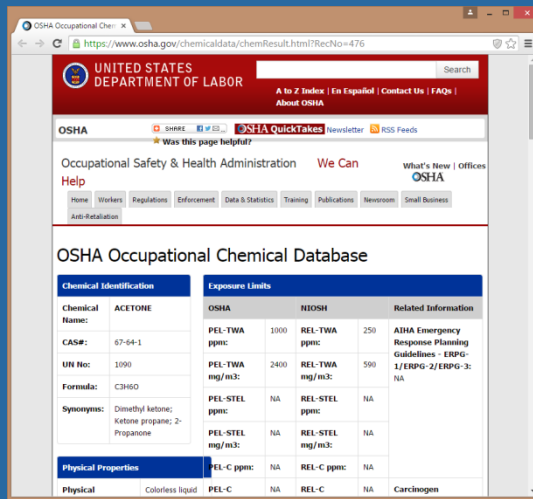
Chemical Name: Dimethyl ketone, ketone propane, 2-Propanone

Chemical ID: 67-64-1

Measurement Methods: NIOSH 1100, 2555, 2880

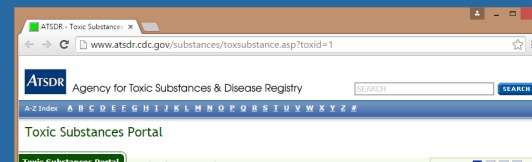
Physical Description: Colorless liquid with a fragrant, mint-like odor.

Flammable Liquid: FLP, below 73°F and BP at or above 100°F.



OSHA Occupational Chemical Database

Chemical Name	Exposure Limits		Related Information
	OSHA	NIOSH	
ACETONE	1000	250	AIHA Emergency Response Planning Guidelines - ERPG-1/ERPG-2/ERPG-3: NA
CAS#:	67-64-1		
UN No:	1090	590	
Formula:	C3H6O		
Synonyms:	Dimethyl ketone; Ketone propane; 2-Propanone		
Physical Properties	REL-C ppvc: NA	REL-C ppvc: NA	
Physical	Colorless liquid	PEL-C NA	REL-C NA Carcinogen

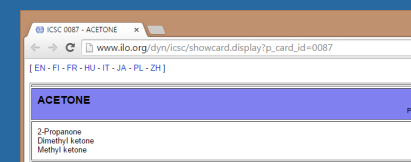


ATSDR - Toxic Substances Portal

Agency for Toxic Substances & Disease Registry

Search

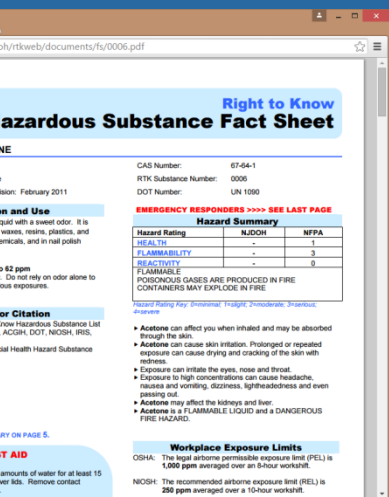
A-Z Index: A B C D E F G H I J K L M N O P Q R S T U V W X Y Z



ICSC 0087 - ACETONE

2-Propanone
Dimethyl ketone
Methyl ketone

One chemical .. many primary sources
Each resource has some overlaps
Each resource has unique content



Hazardous Substance Fact Sheet

Right to Know

CAS Number: 67-64-1

RTK Substance Number: 0006

DOT Number: UN 1590

EMERGENCY RESPONDERS >>>> SEE LAST PAGE

Hazard Rating	NIOSH	MFPA
HEALTH	1	1
FLAMMABILITY	3	3
REACTIVITY	0	0

FLAMMABLE
PERSONAL GASES ARE PRODUCED IN FIRE
CONTAINERS MAY EXPLODE IN FIRE

Acetone can affect you when inhaled and may be absorbed through the skin.

Acetone can cause skin irritation. Prolonged or repeated exposure can cause drying and cracking of the skin with exposure.

Exposure can irritate the eyes, nose and throat.

Exposure to high concentrations can cause headache, nausea and vomiting, dizziness, lightheadedness and even passing out.

Acetone may affect the kidneys and liver.

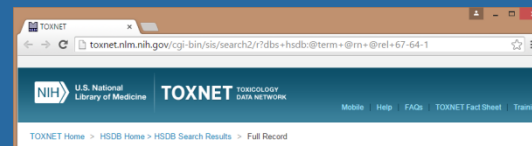
Acetone is a FLAMMABLE LIQUID and a DANGEROUS FIRE HAZARD.

Workplace Exposure Limits

OSHA: The legal airborne permissible exposure limit (PEL) is 1,000 ppm averaged over an 8-hour workshift.

NIOSH: The recommended airborne exposure limit (REL) is 250 ppm averaged over a 10-hour workshift.

Acetone .. seven sources
CDC NIOSH, NJ HSFS, DOL
OSHA, WHO ICSC, NLM
HSDB, EPA ATSDR, EPA/
NOAA CAMEO



TOXNET

U.S. National Library of Medicine

TOXICOLOGY DATA NETWORK

TOXNET Home > HSDB Home > HSDB Search Results > Full Record



CAMEO Chemicals

Chemical Datasheet

ACETONE

What if you have ten chemicals?
What if you have ten sources for each?
How much time will one spend reading them?



Environmental Fate & Exposure

Regulations

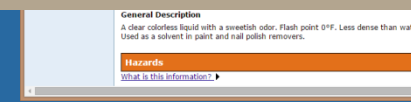
Chemical/Physical Properties

Chemical Safety & Handling

Occupational Exposure Standards

Manufacturing/Use Information

Human Health Effects



General Description

A clear colorless liquid with a sweetish odor. Flash point 0°F. Less dense than water. Used as a solvent in paint and nail polish removers.

Hazards

What is this information?

PubChem Laboratory Chemical Safety Sheet (LCSS)

Pull in primary chemical health and safety resources (as-is possible)

Organize it

Make it available

• Interactive

• In bulk

• On-demand

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

3.3 Boiling Point

56.05 deg C at 760 mm Hg

56 °C

133 °F

133 °F (at 760 mmHg)
(NTP, 1992)

from NIOSH-PocketGuide, OSHA Occupational Chemical DB

from CAMEO Chemicals

LCSS consolidates available health and safety data

- enables rapid cross examination (agreement?)
- fills in information gaps between resources

Source Name: NIOSH-PocketGuide
Source ID: npgd0004
Record Name: Acetone
URL: <http://www.cdc.gov/niosh/npg/npgd0004.html>

Source Name: OSHA Occupational Chemical DB
Source ID: 476
Record Name: ACETONE
URL: <http://www.osha.gov/chemicaldata/chemResult.html?RecNo>

Examples

- Acetone
- Benzene
- Ethanol
- Formald
- Hydroge
- Imidazol
- Phenolpl
- Phosphc
- Theophy
- Toluene

133 °F (at 760 mmHg)
(NTP, 1992)

from CAMEO

9 Stability and Reactivity

10 Storage and Handling

11 Cleanup and Disposal

Signal: Dn

Health and Safety Information summaries are for human

Yes, this is obvious .. and they are great! Succinct write-ups. What more can one ask for?!

Part of a CAMEO record for Acetone

Fire Hazard

Excerpt from [GUIDE 127](#) [Flammable Liquids (Polar / Water-Miscible)]:

HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors may form mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors lighter than air. They will spread along ground and collect in low or confined areas (sewers, basements, tanks). Vapor explosion hazard indoors, outdoors or in sewers. Those substances designated (P) may polymerize explosively when heated or involved in a fire. Runoff to sewer may create explosion hazard. Containers may explode when heated. Many liquids are lighter than water. (2012)

Health Hazard

INHALATION: vapor irritating to eyes and mucous membranes; acts as an anesthetic at high concentrations. **INGESTION:** low order of toxicity but very irritating to mucous membranes; prolonged excessive contact causes defatting of the skin, possibly leading to dermatitis. (1999)

Reactivity Profile

It was reported that a mixture of ACETONE and chloroform, in a residue bottle, exploded on addition of acetone to chloroform in the presence of base will result in a highly exothermic reaction; it is thought that a base was in the bottle [MCA Case History 1661. 1970]. Also, Nitrosyl perchlorate sealed in a tube with a residue of acetone in the presence of platinum catalyst, gave a violent reaction [Chem. Eng. News 35(43):60. 1967]. The reaction of nitrosyl perchlorate and acetone ignites and explodes. Explosions occur with mixtures of nitrosyl perchlorate and primary amines [Ann. Chem. 42:2031. 1909]. Reacts violently with nitric acid. Also causes exothermic reaction when in contact with aldehydes.



Human understanding

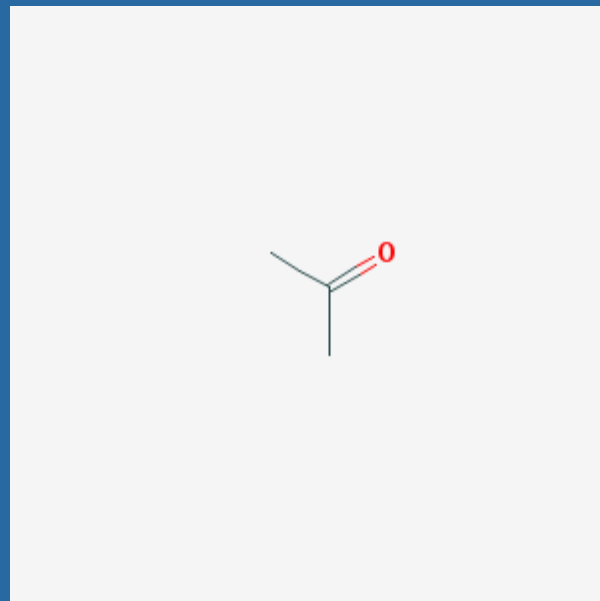
As a chemist, you can understand
and recognize that this picture is the
chemical acetone

You can put a name or registry
number next to it

Is this not good enough?

The picture has no association with
the name or registry number

The computer 'sees' a binary image



Acetone

67-64-1



Computer understanding

Give a computer a chemical

structure a (n)
understand it

Computer can
the structure

Computer can
to the structure

Computer can generate other key
information from structure

propan-2-one
58.07914 g/mol

Computer understanding can help
provide human understanding

If the computer understands, we
can leverage it for search, analysis,
and more



Acc
67



Health and Safety Information summaries for computers

Can human readable
made computer un

Potential workflow involving Computers and Humans

- Humans need to provide the terms and organize them
- Computer can recognize these terms (NER)
- Identify relationships between terms (Human/NLP)
- Relationships fed back to computer
- Harmony ensues .. better navigation, search, analysis

Health Hazard

IRITATION: vapor irritating to eyes and mucous membranes; acts as an anesthetic in very high concentrations. INGESTION: low order of toxicity but very irritating to mucous membranes. Inhaled excess (US)

Sounds good but how?

Computers are not very good at this (yet)

BUT computers combined with humans might be able to do something useful

form, in a residue bottle, exploded. The explosion will result in a highly exothermic reaction [see history 1661. 1970]. Also, Nitrosyl perchlorate, in the presence of platinum catalyst, gave a reaction of nitrosyl perchlorate and nitrosyl perchlorate and primary nitrosyl perchlorate and primary nitrosyl perchlorate. Also causes exothermic

when in contact with aldehydes.



Working with chemical information has CAVEATS!

Chemical information is a bit of a mess and can be rather nuanced

- Names, names, and more names (210M in PubChem)
 - Some standard names are not open and cannot be used/verified without \$\$\$
- Name/structure associations vary by use case (many overlapping)
 - Acetic acid vs. Acetic acid tri-hydrate
 - Formaldehyde: (gas) vs. Formalin (liquid , 40% formaldehyde w/ water)
 - Sulfuric acid: SO_3 (gas) vs. H_2SO_4 (liquid)
 - Glucose: L/D, ring open/closed, alpha/beta/both vs. Glucose monohydrate
 - Large corpus in the 'wild' .. data source dependent nuances

Verify with primary source(s) prior to information use

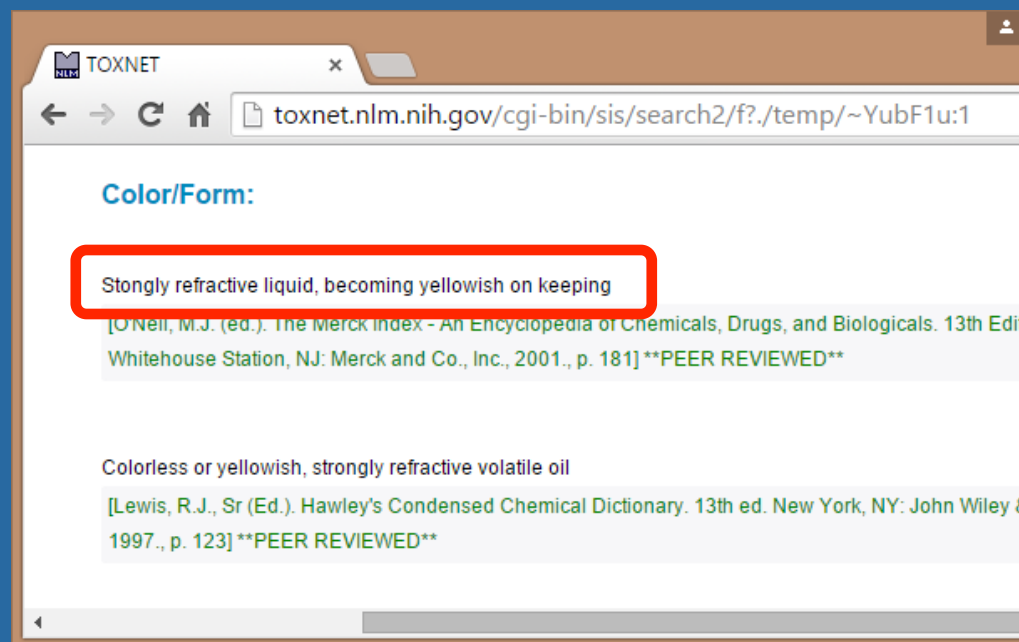
- i.e., is this the form of the chemical I care about?



Working with chemical information has CAVEATS!

Chemical annotation in PubChem is text locked (i.e., meant for humans)

- Benzaldehyde
 - Color
 - Stongly refractive liquid, becoming yellowish on keeping
 - Colorless or yellowish, strongly refractive volatile oil
 - Boiling point
 - 179 deg C
 - 179 °C
 - 354 °F (at 760 mmHg)
 - Flash point
 - 145 deg F, 63 deg C (Closed cup)
 - 73.9 deg C (Open cup)
 - 63 °C



TOXNET

toxnet.nlm.nih.gov/cgi-bin/sis/search2/f?./temp/~YubF1u:1

Color/Form:

Stongly refractive liquid, becoming yellowish on keeping

[O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition. Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 181] **PEER REVIEWED**

Colorless or yellowish, strongly refractive volatile oil

[Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, 1997., p. 123] **PEER REVIEWED**



How can PubChem help?

Well .. we have lots of data

Eureka!!!

Let's Make a connected graph of knowledge

Compound Summary for CID 1140

10.1 Safety and Hazard Identification

10.1.2 Exposure Routes

10.1.3 Symptoms

10.1.4 Target Organs

10.1.5 Fire Hazard

10.1.6 Explosion

10.1.7 Skin Hazard

10.1.8 Inhalation

10.1.9 Eye Hazard

10.1.10 Ingestion

10.1.11 Fire Potential

10.1.12 Skin, Eye, and Respiratory Irritation

10.2 Safety and Hazard

This text can be a useful annotation to ontology.

What if this annotation is provided back to PubChem? It could be used to power more intelligent data integration, access and analysis... for all to use.

safety ontology?

mostly community chemical

10.1.2 Exposure Routes

The substance can be absorbed into the body by inhalation through the skin and by ingestion from ILO-TCSC [9]

inhalation, skin absorption, ingestion, skin and/or eye contact from NIOSH-PocketGuide [10]



What is a knowledge graph?

Knowledge graphs could be envisaged as a network of all kind things which are relevant to a specific domain or to an organization.

<https://blog.semantic-web.at/2014/07/15/from-taxonomies-over-ontologies-to-knowledge-graphs/>



Why a knowledge graph?

(To be) able to make complex queries over the entirety of all kind of information. By breaking up the data silos there is a high probability that query results become more valid.

<https://blog.semantic-web.at/2014/07/15/from-taxonomies-over-ontologies-to-knowledge-graphs/>



end towards community based annotation

“Chemical Safety Ontology” (CSO) participants request and examine a provided table of contents of chemical safety information in PubChem to identify areas of interest

PubChem provides text for a given area of interest to CSO to train the ontology by adding appropriate concepts:

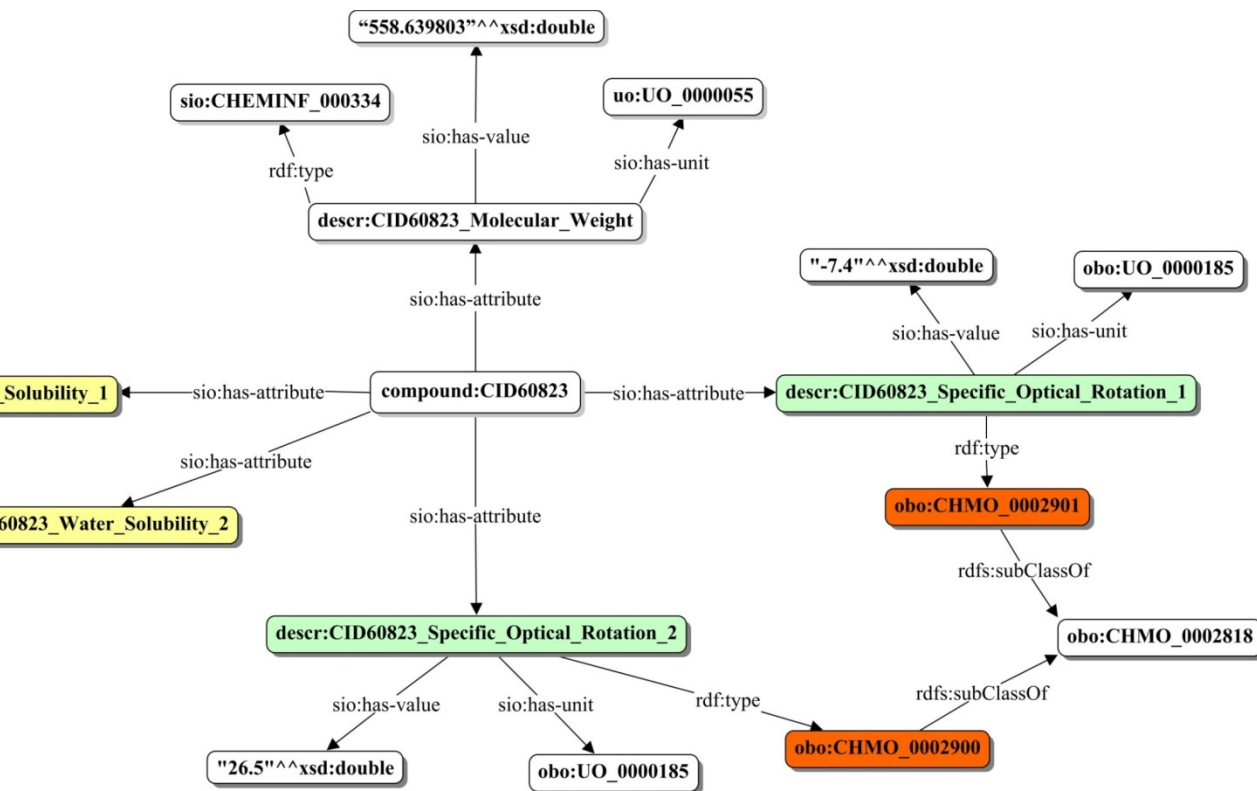
1. PubChem uses current set of ontology terms to auto-annotate the text
2. CSO manually reviews the auto-annotation for ontological gaps, makes fixes
3. Iterate

PubChem may be able to provide tools that help to automate this iterative process and could even serve as a locus for volunteers to semi-manually annotate chemical safety text

PubChem may be able to act as a repository for annotation

- Integration into the PubChemRDF project





Print Share Help

from DrugBank [19]

1), 1.23 mg/mL (pH 6.0) from DrugBank [19]

from DrugBank [19]

from DrugBank [19]

4.2.4 Other Experimental Properties

MW: 1155.36. Specific optical rotation at 25 deg C for D (sodium) line = -7.4 deg (c = 1 in DMSO) /Calcium salt/

O'Neil, M.J. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 148

from HSDB [27]

pKa= 4.46. Solubility in water (30 deg C) = 20.4 ug/ml (pH 2.1); 1.23 mg/ml (pH 6.0) /Sodium salt/

O'Neil, M.J. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 148

from HSDB [27]

MW: 540.62. MP: 159.2-160.7 deg C. Specific optical rotation at 25 deg C = +26.05 (c = 1 in chloroform) /Lactone/

O'Neil, M.J. (ed.). *The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals*. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 148

from HSDB [27]

12 Literature

13 Patents

14 Biomolecular Interactions and Pathways

15 Biological Test Results

16 Classification

17 Information Sources

Chemical Reactivity

Many scenarios of acute interest

- Reaction planning
 - Anything to worry about? Proper protective clothing? Explosion hazards? Incompatibilities? Risks? Storage? Solvent incompatibility? Etc.

Chemical reactivity classification

- NOAA Chemical Reactivity Worksheet (CRW)
- Brethericks
- Knowledge base variants – CAMEO (CRW)

Wouldn't it be great to classify all of PubChem?

- Imagine tools where you could determine incompatibilities for any arbitrary chemical reaction and get an automated assessment



Summary

PubChem provides chemical health and safety information LCSS for chemicals

- Clear provenance of information provided
- Assembling health and safety information for easy access
- Breadth and depth of available information varies greatly per chemical

Chemical information is (sadly) messy

- PLEASE double check the information that it deals with the same thing

Working with chemical health and safety community towards:

- Adding structure to textual data to make it computable
- Chemical reactivity classification



PubChem Crew ...

Steve Bryant

Jie Chen

Tiejun Chen

Gang Fu

Renata Geer

Asta Gindulyte

Lianyi Han

Jane He

Siqian He

Sunghwan Kim

Ben Shoemaker

Paul Thiessen

Jiyao Wang

Yanli Wang

Bo Yu

Jian Zhang

Special thanks to the NCBI Help Desk, especially Rana M



Have any
questions?



Chemical information is everywhere

benzaldehyde

About 700,000 results (0.30 seconds)

Benzaldehyde - Wikipedia, the free encyclopedia
en.wikipedia.org/wiki/Benzaldehyde
Benzaldehyde (C₆H₅CHO) is an organic compound consisting of a benzene ring with a formyl substituent. It is the simplest aromatic aldehyde and one of the ...
Production - Occurrence - Reactions - Uses

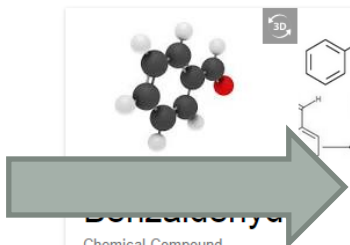
benzaldehyde | C₇H₆O - PubChem
pubchem.ncbi.nlm.nih.gov/compound/benzaldehyde
benzaldehyde | C₇H₆O | CID 240 - structure, chemical names, physical and chemical properties, classification, patents, literature, biological activities, ...

Benzaldehyde | C₇H₆O | ChemSpider
www.chemspider.com/Chemical-Structure.235.html
Structure, properties, spectra, suppliers and links for: Benzaldehyde, 100-52-7.

Benzaldehyde purified by redistillation, ≥99.5% | Sigma ...
www.sigmaaldrich.com/catalog/product/.../418099?
Sigma-Aldrich offers Aldrich-418099, Benzaldehyde for your research needs. Find product specific information including CAS, MSDS, protocols and references.

Benzaldehyde - Britannica.com
www.britannica.com/.../benzaldehyde-C6H5CH...
benzaldehyde (C₆H₅CHO), the simplest representative of the aromatic aldehydes, occurring naturally as the glycoside amygdalin. Prepared synthetically, it is ...

benzaldehyde - Britannica.com
www.britannica.com/science/benzaldehyde
benzaldehyde (C₆H₅CHO), the simplest representative of the aromatic aldehydes, occurring naturally as the glycoside amygdalin. Prepared synthetically, it is ...



PubChem | OPEN CHEMISTRY DATABASE

Search Compounds

Compound Summary for CID 240

Benzaldehyde

Vendors | Drug Information | Pharmacology | Literature | Patents | Bioactivities

	PubChem CID: 240
	Chemical Names: benzaldehyde; Benzoic aldehyde; Benzenecarbonal; Phenylmethanal; 100-52-7; Benzenecarboxaldehyde; More...
	Molecular Formula: C ₇ H ₆ O
	Molecular Weight: 106.12194 g/mol
	InChI Key: HUMNYLRZRPJDN-UHFFFAOYSA-N
	UNII: TA269SD04T
	Modify Date: 2015-06-13
	Create Date: 2004-09-16

Contents

1 2D Structure



Benzaldehyde as a case study

benzaldehyde | C7H6O - F x

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

NLM National Center for Biotechnology Information

Compound Summary for CID 240

Download Print Share Help

18 Information Sources

1. **BENZALDEHYDE from HSDB 388**
2. EPA Chemical Data Report 100-52-7
3. BENZALDEHYDE from ILO-ICSC 0102
Peer-Review Status: 05.04.2006 Validated
4. ECHA 202-860-4
5. Wiki 7076
6. FDA/SPL Indexing data TA269SD04T
7. REGULATION (EC) No 1272/2008 605-012-00-51
8. CAMEO Chemicals CBNOAA00000000000216
9. PubChem
Data deposited in or computed by PubChem
10. benzaldehyde from MeSH 67032175
11. MeSH Tree from MeSH DescTree
MeSH (Medical Subject Headings) is the NLM controlled vocabulary thesaurus used for indexing articles for PubMed.
12. ChEBI Ontology from ChEBI OBO
The ChEBI Ontology is a structured classification of the entities contained within ChEBI.
13. biological process from Gene Ontology GO_ROOT_486550
The Gene Ontology (GO) project provides a controlled vocabulary of terms for describing the functions of gene products, and is divided into three domains. Each term in the biological processes domain, shown here, represents recognized series of events, or a collection of molecular events with a defined beginning and end. Mutant phenotypes often reflect disruptions in biological processes. The terms below apply to the **gene/protein target(s) tested by the BioAssay**.
14. cellular component from Gene Ontology GO_ROOT_486551
The Gene Ontology (GO) project provides a controlled vocabulary of terms for describing the functions of gene products, and is divided into three

benzaldehyde | C7H6O - F x

<https://pubchem.ncbi.nlm.nih.gov/compound/benzaldehyde#section=Top>

Compound Summary for CID 240 2004-09-16

Download Print 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 Drug and Medication Information
- 8 Pharmacology and Biochemistry
- 9 Use and Manufacturing
- 10 Identification
- 11 Safety and Hazards
- 12 Toxicity
- 13 Literature
- 14 Patents
- 15 Biomolecular Interactions and Pathways
- 16 Biological Test Results
- 17 Classification
- 18 Information Sources

1 2D Structure

Search Download Get Image

Magnify

from PubChem

2 3D Conformer

PubChem Compound TOC - Experimental Properties

Physical Description

Color

Form

Color

State

Boiling Point

Melting Point

Flash Point

Solubility

Density

Vapor Density

Vapor Pressure

logP

logS

Henry's Law Constant

Atmospheric OH Rate

Constant

Stability

Optical Rotation

Auto-Ignition

Decomposition

Viscosity

Corrosivity

Volatility

Heat of Combustion

Heat of Vaporization

pH

Surface Tension

Evaporation Rate

Ionicity

Dispersion

Polymerization

Odor Threshold

Enthalpy of Formation

Entropy of Formation

Thermal Conductivity

Electrical Conductivity

Heat of Capacity

Bioavailability

Ghose Filter

Hydrophobicity

Isoelectric Point

Polarizability

Refractive Index

Caco2 Permeability

pKa

pKb

Dissociation Constants

Relative Evaporation Rate

Other Experimental Properties

...



Benzaldehyde chemical and physical properties

The image displays two overlapping browser windows. The background window is the PubChem Compound Summary for Benzaldehyde (CID 240), with the 'Flash Point' section selected in the left-hand 'Contents' menu. The foreground window is a ToxNet search result for benzaldehyde, which is linked to the PubChem page. An arrow points from the 'Flash Point' section in the foreground window to a callout box containing detailed information.

PubChem Compound Summary for CID 240

- Contents
 - 4 Chemical and Physical Properties
 - 4.1 Computed Properties
 - 4.2 Experimental Properties
 - 4.2.1 Physical Description
 - 4.2.2 Color
 - 4.2.3 Odor
 - 4.2.4 Taste
 - 4.2.5 Boiling Point
 - 4.2.6 Melting Point
 - 4.2.7 Flash Point**
 - 4.2.8 Solubility
 - 4.2.9 Density
 - 4.2.10 Vapor Density
 - 4.2.11 Vapor Pressure
 - 4.2.12 LogP
 - 4.2.13 Stability
 - 4.2.14 Auto-Ignition

4.2.7 Flash Point

145 deg F, 63 deg C (Closed cup)
Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, 1997., p. 325-16
from HSDB

Source Name: HSDB
Source ID: 388
Record Name: BENZALDEHYDE
URL: <http://toxnet.nlm.nih.gov/cgi-bin/sis/search/r?dbs+hsdb:@term+@m+@rel+100-52-7>

73.9 deg C (Open cup)
Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984., p. V3 737 (1978)
from HSDB

63 °C
from ILO-ICSC

4.2.8 Solubility

Approximately 0.6% wt. at 20 deg C
Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. V4: 64 (1992)
from HSDB

Miscible with alcohol, ether, fixed and volatile oils
Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 123

ToxNET Search Results

Flash Point:

145 deg F, 63 deg C (Closed cup)
[Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, 1997., p. 325-16] **PEER REVIEWED**

73.9 deg C (Open cup)
[Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984., p. V3 737 (1978)] **PEER REVIEWED**

Autoignition Temperature:

377 deg F, 192 deg C
[Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, 1997., p. 325-16] **PEER REVIEWED**

Fire Fighting Procedures:

If material on fire or involved in fire: Do not extinguish fire unless fire is under control. Use water in flooding quantities as fog. Solid streams of water may be ineffective. Apply water from as far a distance as possible. (Association of American Railroads/Bureau of Explosives, Emergency Response Team, Association of American Railroads, Pueblo, CO, 2002)

PubChem Compound Table of Contents

PubChem Classification Browser

PubChem

Search selected

Keyword

Classification description (from PubChem)

Classification was created automatically from the PubChem Compound Table of Contents. It includes all chemical substances in the PubChem Compound Table of Contents, along with their child subsections, that are not shown in the PubChem Compound Table of Contents. It includes all chemical substances in the PubChem Compound Table of Contents with Annotation, Related Substances, 2D Structure, 3D Structure, and 3D Status.

Type counts to display

one Compound

Use PubChem Tree

- PubChem Compound TOC ?
- Biological Test Results ?
- Biomolecular Interactions and Pathways ?
- Chemical and Physical Properties ?

PubChem Compound TOC ? 25,341,688

- Biological Test Results ? 2,083,799
- Biomolecular Interactions and Pathways ? 42,078
- Chemical and Physical Properties ? 13,123
 - Experimental Properties ? 13,102
 - Spectral Properties ? 4,949
- Classification ? 14,005,879
- Drug and Medication Information ? 6,425
- Identification ? 200,235
- Literature ? 325,799
- Patents ? 16,701,075
- Pharmacology and Biochemistry ? 18,651
- Related Records ? 4,745,630
- Safety and Hazards ? 8,867
- Toxicity ? 9,031
- Use and Manufacturing ? 7,291
- 3D Status ? 5,839,251

You are here: NCBI > Chemicals & Bioassays > PubChem > Classification Browser

GETTING STARTED RESOURCES POPULAR FEATURED NCBI INFORMATION

HSDB is very high quality and peer reviewed (\$\$\$); however, it is limited to ~5800 chemical substances

To extend coverage, sources of additional authoritative information added to PubChem

Facebook Twitter Google+

- BioActivity Summary
- BioActivity Databank
- BioActivity SAR
- BioActivity Data Dictionary
- Structure Search
- 3D Conformer Tools
- Structure Clustering
- Classification
- Upload
- Download
- PubChem FTP

OSHA SDS (Safety Data Sheet, formerly MSDS) standard

The image shows two overlapping browser windows from PubChem. The left window displays a search for "benzaldehyde" with 1 result. Below the search, a "Chem Tree (filter applied)" is shown with a list of experimental properties, each with a question mark icon and a count of 1. A red arrow points from the search results in the right window to the "Experimental Properties" section in the left window.

PubChem Classification Browser

Search selected classification by: PubChem Keyword Enter desired search term

Description (from PubChem): Information was created automatically from the PubChem Compound TOC on 2015/05/13. 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 along with their child subsections, that are not shown in this tree are: Computed Properties, Substance Categorization Classification, Depositor-Supplied Synonyms, Removed Synonyms, Create Date, Modify Date, Record Title, Related Compounds, Related Compound Annotation, Related Substances, 2D Structure, 3D Conformer, and Chemical Vendors. More...

Items to display: Display zero count nodes? Filter by Entrez History

#7 Search "benzaldehyde"[completesynonym] (pccompound): 1 results

Choose one

- #7 Search "benzaldehyde"[completesynonym] (pccompound): 1 results
- #6 Search "benzaldehyde" (pccompound): 64723 results
- #4 Search (#3) (pccompound): 1812 results
- #3 Select 1812 document(s) (pccompound): 1812 results
- #5 Select 1283 document(s) (pccompound): 1283 results
- #2 Search (#1) (pccompound): 2704 results
- #1 Select 2704 document(s) (pccompound): 2704 results

Chem Tree (filter applied)

- Chemical and Physical Properties ? 1
- Biological Test Results ? 1
- Biomolecular Interactions and Pathways ? 1
- Experimental Properties ? 1
 - Auto-Ignition ? 1
 - Boiling Point ? 1
 - Color ? 1
 - Density ? 1
 - Dissociation Constants ? 1
 - Flash Point ? 1
 - Heat of Combustion ? 1
 - Heat of Vaporization ? 1
 - LogP ? 1
 - Melting Point ? 1
 - Odor ? 1
 - Odor Threshold ? 1
 - Other Experimental Properties ? 1

Section 16. Other information