

Chemical Safety Data Sheet MSDS / SDS

4-hydroxy-4-methylpentan-2-one SDS

Revision Date:2024-04-25 Revision Number:1

Section 1	Section 2	Section 3	Section 4	Section 5	Section 6	Section 7	Section 8
Section 9	Section 10	Section 11	Section 12	Section 13	Section 14	Section 15	Section 16

SECTION 1: Identification of the substance/mixture and of the company/undertaking**Product identifier**

Product name: 4-hydroxy-4-methylpentan-2-one

CAS: 123-42-2

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses: For R&D use only. Not for medicinal, household or other use.

Uses advised against: none

Company Identification

Company: Chemicalbook.in

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

Telephone: +91 9550333722

SECTION 2: Hazards identification**Classification of the substance or mixture**

Eye irritation, Category 2

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

Hazard statement(s)

H319 Causes serious eye irritation

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

Response

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Storage

none

Disposal

none

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name: 4-hydroxy-4-methylpentan-2-one

Common names and synonyms: 4-hydroxy-4-methylpentan-2-one

CAS number: 123-42-2
EC number: 204-626-7
Concentration: 100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap.

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Do NOT induce vomiting. Give one or two glasses of water to drink. Refer for medical attention .

Most important symptoms/effects, acute and delayed

Vapor is irritating to the mucous membrane of the eye and respiratory tract. Inhalation can cause dizziness, nausea, some anesthesia. Very high concentrations have a narcotic effect. The liquid is not highly irritating to the skin but can cause dermatitis. (USCG, 1999)

Indication of immediate medical attention and special treatment needed, if necessary

Absorption, Distribution and Excretion

Absorption ... occurs readily from the lung.

SECTION 5: Firefighting measures

Suitable extinguishing media

Alcohol foam, foam, carbon dioxide, dry chemical .

Specific hazards arising from the chemical

Excerpt from ERG Guide 129 [Flammable Liquids (Water-Miscible / Noxious)]: HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors are heavier 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 with a (P) may polymerize explosively when heated or involved in a fire. Runoff to sewer may create fire or explosion hazard. Containers may explode when heated. Many liquids are lighter than water. (ERG, 2016)

Special protective actions for fire-fighters

Use water spray, alcohol-resistant foam, dry powder, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Remove all ignition sources. Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Cover the spilled material with inert absorbent. Carefully collect remainder.

Environmental precautions

Remove all ignition sources. Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Cover the spilled material with inert absorbent. Carefully collect remainder.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. Above 58°C use a closed system, ventilation and explosion-proof electrical equipment. Use non-sparking handtools. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and

eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Fireproof. Separated from acids, bases, amines and oxidants... MATERIALS WHICH ARE TOXIC AS STORED OR WHICH CAN DECOMPOSE INTO TOXIC COMPONENTS ... SHOULD BE STORED IN A COOL WELL-VENTILATED PLACE, OUT OF THE DIRECT RAYS OF THE SUN, AWAY FROM AREAS OF HIGH FIRE HAZARD, AND SHOULD BE PERIODICALLY INSPECTED ... INCOMPATIBLE MATERIALS SHOULD BE ISOLATED .

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 50 ppm as TWA.MAK: 96 mg/m³, 20 ppm; peak limitation category: I(2); skin absorption (H); pregnancy risk group: D

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear safety goggles.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Liquid.
Colour:	COLORLESS LIQUID
Odour:	FAINT PLEASANT ODOR
Melting point/freezing point:	-44 °C.
Boiling point or initial boiling point and boiling range:	167.9 °C. Atm. press.:760 Torr.
Flammability:	Class II Combustible Liquid: Fl.P. at or above 100°F and below 140°F.
Lower and upper explosion limit/flammability limit:	1.8% LOWER & 6.9% UPPER
Flash point:	63.5 °C. Atm. press.:101.3 kPa.;62.5 °C. Atm. press.:101.3 kPa.;61 °C. Atm. press.:101.3 kPa.
Auto-ignition temperature:	643 °C. Atm. press.:1.013 atm. Remarks:Atmospheric pressure is not reported. An atm pressure is only added for TCC reasons.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	dynamic viscosity (in mPa s) = 28.7. Temperature:-25.0°C.;dynamic viscosity (in mPa s) = 6.621. Temperature:0.0°C.;dynamic viscosity (in mPa s) = 2.798. Temperature:25.0°C.
Solubility:	Miscible with water
Partition coefficient n-octanol/water:	log Pow = 1.9. Remarks:Temperature was not reported.
Vapour pressure:	1 mm Hg. Temperature:68 °F. Remarks:Reported as 1 mm Hg at 68oF.;1.35 hPa. Temperature:20 °C. Remarks:Converted from the value in mmHg and °F.

Density and/or relative density:	0.9 a relative density doesn't have unit. Temperature:20 °C.
Relative vapour density:	4 (vs air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

1800 ppm [Based on 10% of the lower explosive limit for safety considerations even though the relevant toxicological data indicated that irreversible health effects or impairment of escape existed only at higher concentrations.]

Decomposes on heating or on burning or on contact with acids, bases and amines. This produces acetone and mesityl alcohol. Reacts violently with oxidants. This produces flammable/explosive gas (hydrogen - see ICSC 0001).

Chemical stability

Decomposed by prolonged exposure to alkalis & by distillation at atmospheric pressure

Possibility of hazardous reactions

MODERATE WHEN EXPOSED TO HEAT OR FLAME ...Acetyl bromide reacts violently with alcohols or water, [Merck 11th ed., 1989]. Mixtures of alcohols with concentrated sulfuric acid and strong hydrogen peroxide can cause explosions. Example: An explosion will occur if dimethylbenzylcarbinol is added to 90% hydrogen peroxide then acidified with concentrated sulfuric acid. Mixtures of ethyl alcohol with concentrated hydrogen peroxide form powerful explosives. Mixtures of hydrogen peroxide and 1-phenyl-2-methyl propyl alcohol tend to explode if acidified with 70% sulfuric acid, [Chem. Eng. News 45(43):73(1967); J. Org. Chem. 28:1893(1963)]. Alkyl hypochlorites are violently explosive. They are readily obtained by reacting hypochlorous acid and alcohols either in aqueous solution or mixed aqueous-carbon tetrachloride solutions. Chlorine plus alcohols would similarly yield alkyl hypochlorites. They decompose in the cold and explode on exposure to sunlight or heat. Tertiary hypochlorites are less unstable than secondary or primary hypochlorites, [NFPA 491 M, 1991]. Base-catalysed reactions of isocyanates with alcohols should be carried out in inert solvents. Such reactions in the absence of solvents often occur with explosive violence, [Wischmeyer(1969)].

Conditions to avoid

no data available

Incompatible materials

Strong oxidizers, strong alkalis.

Hazardous decomposition products

When heated to decomp it emits acrid smoke and fumes.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male/female) - 3 002 mg/kg bw.

Inhalation: LC0 - rat (male/female) - ≥ 7.6 mg/L air.

Dermal: LD0 - rat (male/female) - $> 1\,875$ mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance is irritating to the eyes, skin and respiratory tract. If this liquid is swallowed, aspiration into the lungs may result in chemical pneumonitis. Exposure far above the OEL could cause lowering of consciousness.

STOT-repeated exposure

The substance defats the skin, which may cause dryness or cracking.

Aspiration hazard

A harmful contamination of the air will not or will only very slowly be reached on evaporation of this substance at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - *Oryzias latipes* - > 100 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - > 1 000 mg/L - 48 h.

Toxicity to algae: EC50 - *Pseudokirchneriella subcapitata* (previous names: *Raphidocelis subcapitata*, *Selenastrum capricornutum*) - > 1 000 mg/L - 72 h.

Toxicity to microorganisms: EC50 - activated sludge, domestic - > 1 000 mg/L - 3 h. Remarks: Respiration rate.

Persistence and degradability

Two sets of tests using acclimated mixed microbial cultures as inoculum gave percent theoretical BOD of 47%(1) and 46%(2) after 5 days for 4-hydroxy-4-methyl-2-pentanone under aerobic conditions(1,2). A percent theoretical BOD of 3% was observed after 5 days in screening tests using the standard dilution technique under aerobic conditions and effluent sewage from a biological sanitary waste treatment plant as inoculum; 31% theoretical BOD was observed after 5 days using adapted effluent sewage(3). No information regarding biodegradation in natural media was found(SRC).

Bioaccumulative potential

An estimated BCF of 0.50 can be calculated(SRC) from an estimated log Kow of -0.098(2) using a recommended regression equation(1). Based upon the estimated BCF and the reported infinite solubility of the compound in water(3), 4-hydroxy-4-methyl-2-pentanone will not be expected to significantly bioconcentrate in aquatic organisms(SRC).

Mobility in soil

An estimated Koc of 21 can be calculated(SRC) from an estimated log Kow of -0.098(2) using a recommended regression equation(1). Based upon the estimated Koc and the reported infinite solubility of the compound in water(3), 4-hydroxy-4-methyl-2-pentanone will not be expected to strongly adsorb to sediment or suspended particulate matter(4,SRC). It will be expected to exhibit very high mobility in soil(4), and therefore, 4-hydroxy-4-methyl-2-pentanone may leach through soil to groundwater if it does not volatilize or biodegrade first(SRC).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN1148 (For reference only, please check.)

IMDG: UN1148 (For reference only, please check.)

IATA: UN1148 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: DIACETONE ALCOHOL (For reference only, please check.)

IMDG: DIACETONE ALCOHOL (For reference only, please check.)

IATA: DIACETONE ALCOHOL (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 3 (For reference only, please check.)

IMDG: 3 (For reference only, please check.)

IATA: 3 (For reference only, please check.)

Packing group, if applicable

ADR/RID: II (For reference only, please check.)

IMDG: II (For reference only, please check.)

IATA: II (For reference only, please check.)

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information**Safety, health and environmental regulations specific for the product in question****European Inventory of Existing Commercial Chemical Substances (EINECS)**

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website:
<http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Other Information

This card is only valid for the pure substance. The technical product may contain up to 5% acetone (see ICSC 0087), resulting in high flammability. Other UN Classification for technical product: UN hazard class 3, UN pack group II.

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any