

Chemical Safety Data Sheet MSDS / SDS

Acetoin SDS

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

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

Product name: Acetoin
CAS: 513-86-0

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

Flammable liquids, Category 3
Serious eye damage, Category 1

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

Hazard statement(s)

H226 Flammable liquid and vapour

H318 Causes serious eye damage

Precautionary statement(s)

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P233 Keep container tightly closed.

P240 Ground and bond container and receiving equipment.

P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.

P242 Use non-sparking tools.

P243 Take action to prevent static discharges.

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

Response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].

P370+P378 In case of fire: Use ... to extinguish.

P305+P354+P338 IF IN EYES: Immediately rinse with water for several minutes. Remove contact lenses, if present and easy to do.

Continue rinsing.

P317 Get medical help.

Storage

P403+P235 Store in a well-ventilated place. Keep cool.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	Acetoin
Common names and synonyms:	Acetoin
CAS number:	513-86-0
EC number:	208-174-1
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms/effects, acute and delayed

Excerpt from ERG Guide 127 [Flammable Liquids (Water-Miscible)]: Inhalation or contact with material may irritate or burn skin and eyes. Fire may produce irritating, corrosive and/or toxic gases. Vapors may cause dizziness or suffocation. Runoff from fire control may cause pollution. (ERG, 2016)

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

Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if needed. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary . Monitor for shock and treat if necessary . Anticipate seizures and treat if necessary . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with normal saline during transport . Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool . Cover skin burns with dry sterile dressings after decontamination . Poison A and B

SECTION 5: Firefighting measures

Suitable extinguishing media

Excerpt from ERG Guide 127 [Flammable Liquids (Water-Miscible)]: CAUTION: All these products have a very low flash point: Use of water spray when fighting fire may be inefficient. CAUTION: For fire involving UN1170, UN1987 or UN3475, alcohol-resistant foam should be used. SMALL FIRE: Dry chemical, CO₂, water spray or alcohol-resistant foam. LARGE FIRE: Water spray, fog or alcohol-resistant foam. Do not use straight streams. Move containers from fire area if you can do it without risk. FIRE INVOLVING TANKS OR CAR/TRAILER LOADS: Fight fire from maximum distance or use unmanned hose holders or monitor nozzles. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks engulfed in fire. For massive fire, use unmanned hose holders or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2016)

Specific hazards arising from the chemical

Excerpt from ERG Guide 127 [Flammable Liquids (Water-Miscible)]: 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

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

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

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

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

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 tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flare resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Acetyl methyl carbinol is a light-yellow colored liquid. Slightly denser than water. Hence sinks in water. Used to make other chemicals.
Colour:	Slightly yellow liquid or crystals
Odour:	Buttery odor
Melting point/freezing point:	106°C(lit.)
Boiling point or initial boiling point and boiling range:	148°C(lit.)
Flammability:	no data available

Lower and upper explosion limit/flammability limit:	no data available
Flash point:	47° C
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	In water: SOLUBLE
Partition coefficient n-octanol/water:	log Kow = -0.36 /Estimated/
Vapour pressure:	2.7X10+0 at 25 deg C /Estimated/
Density and/or relative density:	1.013g/mL at 25° C (lit.)
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Flammable. Slightly soluble in water.

Chemical stability

Forms a solid dimer C₈H₁₆O₄ on standing or on treatment with granulated zinc. The dimer is easily converted back to the monomer by melting, distilling, or dissolving.

Possibility of hazardous reactions

Flammable liquid ACETYL METHYL CARBINOL is a ketone and alcohol. Ketones are reactive with many acids and bases liberating heat and flammable gases (e.g., H₂). The amount of heat may be sufficient to start a fire in the unreacted portion of the ketone. Ketones react with reducing agents such as hydrides, alkali metals, and nitrides to produce flammable gas (H₂) and heat. Ketones are incompatible with isocyanates, aldehydes, cyanides, peroxides, and anhydrides. They react violently with aldehydes, HNO₃, HNO₃ + H₂O₂, and HClO₄. Flammable and/or toxic gases are generated by the combination of alcohols with alkali metals, nitrides, and strong reducing agents. They react with oxoacids and carboxylic acids to form esters plus water. Oxidizing agents convert them to aldehydes or ketones. Alcohols exhibit both weak acid and weak base behavior. They may initiate the polymerization of isocyanates and epoxides.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and fumes.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD₅₀ Rat oral >5000 mg/kg bw from table

Inhalation: no data available

Dermal: no data available

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

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information**Toxicity**

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: Three activated sludges from Columbus, Hilliard, and Linwood, OH wastewater treatment plants were used as inocula in Warburg respirometer tests designed to measure oxygen uptake of acetoin(1). The suspended solids concentration was adjusted to 2,500 mg/L; acetoin was added to obtain a concentration of 500 mg/L and incubated at 20 deg C. Average theoretical BOD values measured at 6, 12 and 24 hours were 2.6, 4.3, and 13.8%, respectively, indicating that biodegradation is an important fate process(1).

Bioaccumulative potential

An estimated BCF of 0.3 was calculated for acetoin(SRC), using a water solubility of 1.0×10^{-6} mg/L(1), and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

The Koc of acetoin is estimated as 2(SRC), using a water solubility of 1.0×10^{-6} mg/L(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that acetoin is expected to have very high mobility in soil.

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: UN2621 (For reference only, please check.)

IMDG: UN2621 (For reference only, please check.)

IATA: UN2621 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: ACETYL METHYL CARBINOL (For reference only, please check.)

IMDG: ACETYL METHYL CARBINOL (For reference only, please check.)

IATA: ACETYL METHYL CARBINOL (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: III (For reference only, please check.)

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

IATA: III (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/>

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