Chemical Safety Data Sheet MSDS / SDS

Methyl acetoacetate 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: Methyl acetoacetate

CAS: 105-45-3

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

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

uses:

Uses advised none

against:

Company Identification

Company: Chemicalbook.in

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

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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: Methyl acetoacetate

Common names and Methyl acetoacetate

synonyms:

CAS number: 105-45-3

EC number: 203-299-8

Concentration: 100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower.

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

May be harmful by inhalation, ingestion, or skin absorption. Causes eye irritation. May cause skin irritation. (USCG, 1999)

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

Use/ foam, carbon dioxide, dry chemical.

Specific hazards arising from the chemical

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]: HIGHLY FLAWWABLE: 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. Substance may be transported hot. For hybrid vehicles, ERG Guide 147 (lithium ion batteries) or ERG Guide 138 (sodium batteries) should also be consulted. If molten aluminum is involved, refer to ERG Guide 169. (ERG, 2016)

Special protective actions for fire-fighters

Use alcohol-resistant foam, powder, carbon dioxide.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Ventilation. Collect leaking and spilled liquid in sealable containers as far as possible. Wash away remainder with plenty of water.

Environmental precautions

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Ventilation. Collect leaking and spilled liquid in sealable containers as far as possible. Wash away remainder with plenty of water.

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. Above 77°C use a closed system and ventilation. 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

Separated from oxidants.

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 safety goggles.

Skin protection

Protective gloves.

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: Methyl acetoacetate is a clear colorless liquid. Flash point 158°F. Denser than water and

slightly soluble in water. Vapors heavier than air.

Colorless liquid

Odour: Agreeable odor

Melting -80°C

point/freezing

point:

Boiling point or 169-170°C

initial boiling point and boiling range:

Flammability: Combustible.

Lower and upper

explosion

limit/flammability

limit:

Flash point: 67°C

Auto-ignition 536° F (USCG, 1999)

temperature:

Decomposition no data available

temperature:

pH: no data available

Kinematic 1.704 cPa at 20 deg C

viscosity:

Solubility: Soluble in 2 parts water; miscible with alcohol and ether

no data available

Partition log Kow = -0.69 /Estimated/

coefficient noctanol/water:

Vapour pressure: 1.54mmHg at 25°C

Density and/or 1.077

relative density:

Relative vapour

4.0 (Air= 1)

density:

Particle

no data available

characteristics:

SECTION 10: Stability and reactivity

Reactivity

Decomposes on burning. This produces irritating fumes. Reacts with oxidants.

Chemical stability

MAA and EAA are stable liquids

Possibility of hazardous reactions

FIRE HAZARD: Moderate, when exposed to heat or flame.METHYL ACETOACETATE is an ester. Esters react with acids to liberate heat along with alcohols and acids. Strong oxidizing acids may cause a vigorous reaction that is sufficiently exothermic to ignite the reaction products. Heat is also generated by the interaction of esters with caustic solutions. Flammable hydrogen is generated by mixing esters with alkali metals and hydrides

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and irritating fumes

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Rat oral 3.0 g/kg

Inhalation: LC50 Rat inhalation >6.6 mg/L/4 hr

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

The substance is irritating to the eyes and respiratory tract. Exposure could cause lowering of consciousness.

STOT-repeated exposure

no data available

Aspiration hazard

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 Pimephales promelas (Fathead minnow) >111.4 mg/L/96 hr; static; temperature ranged from 19-20 deg C, pH ranged from 7.7 to 8.4 and dissolved oxygen ranged from 7.8 to 9.1 mg/L.

Toxicity to daphnia and other aquatic invertebrates: EC50 Daphnia magna (Water flea; Acute immobilization test and reproduction) >236.9 mg/L/48 hr; static; exposure temperature ranged from 20-21 deg C, pH ranged from 7.9 to 8.3, and dissolved oxygen ranged from 8.7 to 8.9 mg/L

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: Methyl acetoacetate, present at 100 mg/L, reached 78% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/L and the Japanese MITI test(1). Methyl acetoacetate was degraded more than 90% in 2 days at 22 deg C using activated sludge inoculum in a Zahn-Wellens screening test(2).

Bioaccumulative potential

An estimated BCF of 3.1 was calculated for methyl acetatoactate(SRC), using an estimated log Kow of -0.69(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

Using a structure estimation method based on molecular connectivity indices(1), the Koc for methyl acetoacetate can be estimated to be 1.0(SRC). According to a classification scheme(2), this estimated Koc value suggests that methyl acetoacetate 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: Not dangerous goods. (For reference only, please check.) IMDG: Not dangerous goods. (For reference only, please check.) IATA: Not dangerous goods. (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.) IMDG: Not dangerous goods. (For reference only, please check.) IATA: Not dangerous goods. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.) IMDG: Not dangerous goods. (For reference only, please check.) IATA: Not dangerous goods. (For reference only, please check.)

Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.) IMDG: Not dangerous goods. (For reference only, please check.) IATA: Not dangerous goods. (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

Not 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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