# Chemical Safety Data Sheet MSDS / SDS

## 5-methylhexan-2-one SDS

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



## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### Product identifier

Product name: 5-methylhexan-2-one

CAS: 110-12-3

### 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

Flammable liquids, Category 3
Acute toxicity - Category 4, Inhalation

## GHS label elements, including precautionary statements

Pictogram(s)

Signal word Warning

### Hazard statement(s)

H226 Flammable liquid and vapour
H332 Harmful if inhaled

### 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/...
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.

### 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.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
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: | 5-methylhexan-2-one |
| Common names and synonyms: | 5-methylhexan-2-one |
| CAS number: | 110-12-3 |
| EC number: | 203-737-8 |
| 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

First rinse with plenty of water for at least 15 minutes, then remove contaminated clothes and rinse again. Refer for medical attention .

### 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. Refer for medical attention .

### 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

INHALATION. Symptoms: Cough. Headache. Dizziness. Drowsiness. Labored breathing. Sore throat. First aid: Fresh air, rest. Refer for medical attention. SKIN: Symptoms: Dry skin. Redness. First aid: First rinse with plenty of water, then remove contaminated clothes and rinse again. Refer for medical attention. EYES: Symptoms: Redness. First aid: First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then take to a doctor. INGESTION: Symptoms: Nausea. First aid: Rinse mouth. Do NOT induce vomiting. Refer for medical attention.

## SECTION 5: Firefighting measures

### Suitable extinguishing media

If material on fire or involved in fire: Do not extinguish fire unless flow can be stopped or safely confined. Use water in flooding quantities as fog. Solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water. Apply water from as far a distance as possible. Use alcohol foam, dry chemical or carbon dioxide. Keep run-off water out of sewers and water sources.

### 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

Use AFFF, alcohol-resistant foam, 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

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Ventilation. Collect leaking liquid in sealable containers. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT wash away into sewer.

### Environmental precautions

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Ventilation. Collect leaking liquid in sealable containers. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT wash away into sewer.

### Methods and materials for containment and cleaning up

Evacuate and restrict persons not wearing protective equipment from area of spill or leak until cleanup is complete. Remove all ignition sources. Establish forced ventilation to keep levels below explosive limit. Absorb liquids in vermiculite, dry sand, earth, peat, carbon, or similar material and deposit in sealed containers. Keep this chemical out of a confined space ... because of the possibility of an explosion ... It may be necessary to contain and dispose of this chemical as a hazardous waste. If material or contaminated runoff enters waterways, notify downstream users of potentially contaminated waters. Contact your Department of Environmental Protection or your regional office of the federal EPA for specific recommendations. If employees are required to clean up spills, they must be properly trained and equipped. OSHA 1910.120(q) may be applicable.

## SECTION 7: Handling and storage

### Precautions for safe handling

NO open flames, NO sparks and NO smoking. Above 36°C use a closed system, ventilation and explosion-proof electrical equipment. 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.... Store in tightly closed containers in a cool, well ventilated area away from sources of oxidizers (such as perchlorates, peroxides, permanganates, chlorates, and nitrates), strong oxidizers (such as chlorine, bromine, and fluorine), reducing agents, and aldehydes. Sources of ignition such as smoking and open flames are prohibited where methyl isoamyl ketone is handled, used or stored. Metal containers involving the transfer of 5 gallons or more of methyl isoamyl ketone should be grounded and bonded. Drums must be equipped with self-closing valves, pressure vacuum bungs, and flame arresters.

## SECTION 8: Exposure controls/personal protection

### Control parameters

### Occupational Exposure limit values

TLV: 20 ppm as TWA; 50 ppm as STEL.MAK: 47 mg/m3, 10 ppm; peak limitation category: I(2); pregnancy risk group: D.EU-OEL: 95 mg/m3, 20 ppm as TWA

**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 spectacles or eye protection in combination with breathing protection.

**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. |
| Odour: | Pleasant, fruity odor |
| Melting point/freezing point: | -73.9 °C. Atm. press.:1 atm. |

| | |
|---|---|
| Boiling point or initial boiling point and boiling range: | 144 °C. Atm. press.:1 atm. |
| Flammability: | Class IC Flammable Liquid: Fl.P. at or above 73°F and below 100°F. |
| Lower and upper explosion limit/flammability limit: | Lower flammable limit: 1.0% by volume @ 200 deg F (93 deg C); Upper flammable limit: 8.2% by volume @ 200 deg F (93 deg C) |
| Flash point: | 36 °C. Atm. press.:101.325 kPa. |
| Auto-ignition temperature: | 400 °C. Atm. press.:1 atm. |
| Decomposition temperature: | no data available |
| pH: | no data available |
| Kinematic viscosity: | dynamic viscosity (in mPa s) = 0.704. Temperature:25.0°C. |
| Solubility: | 0.5 % (NIOSH, 2016) |
| Partition coefficient n-octanol/water: | log Pow = 1.94. Temperature:25 °C. |
| Vapour pressure: | 665 Pa. Temperature:25 °C. |
| Density and/or relative density: | 0.81 g/cm3. Temperature:20 °C. |
| Relative vapour density: | 3.94 (vs air) |
| Particle characteristics: | no data available |

## SECTION 10: Stability and reactivity

**Reactivity**

Reacts violently with strong oxidants, strong bases, amines and isocyanates. This generates fire and explosion hazard. Attacks some

plastics.

### Chemical stability

Stable containers: drums; tank cars

### Possibility of hazardous reactions

FlammableThe vapour mixes well with air, explosive mixtures are easily formed.Ketones, such as 5-METHYLHEXAN-2-ONE, 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.

### Conditions to avoid

no data available

### Incompatible materials

The vapor mixes well with air, explosive mixtures are easily formed.

### Hazardous decomposition products

When heated to decomposition it emits acrid smoke and irritating fumes.

## SECTION 11: Toxicological information

### Acute toxicity

Oral: LD50 - rat (male) - 5 657 mg/kg bw. Remarks:The two highest dose levels (4000 and 8000 mg/kg bw) used in this study were higher than that used for a limit dose in present-day guideline studies.

Inhalation: LC50 - rat (male) - > 3 207 - < 5 875 ppm.

Dermal: LDLo - guinea pig - > 10 mL/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. The substance may cause effects on the kidneys. This may result in kidney impairment. Exposure above the OEL could cause lowering of consciousness.

### STOT-repeated exposure

Repeated or prolonged contact with skin may cause dermatitis.

### Aspiration hazard

A harmful contamination of the air will be reached rather slowly on evaporation of this substance at 20°C; rather slowly.

## SECTION 12: Ecological information

### Toxicity

Toxicity to fish: LC50 - Pimephales promelas - 159 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - > 100 mg/L - 48 h.

Toxicity to algae: EC50 - Pseudokirchneriella subcapitata (previous names: Raphidocelis subcapitata, Selenastrum capricornutum) - > 100 mg/L - 72 h.

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

### Persistence and degradability

no data available

### Bioaccumulative potential

An estimated BCF of 6 was calculated in fish for 5-methyl-2-hexanone(SRC), using a log Kow of 1.88(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 5-methyl-2-hexanone is estimated as 250(SRC), using a log Kow of 1.88(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that 5-methyl-2-hexanone is expected to have moderate 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: UN2302 (For reference only, please check.)
IMDG: UN2302 (For reference only, please check.)
IATA: UN2302 (For reference only, please check.)

### UN Proper Shipping Name

ADR/RID: 5-METHYLHEXAN-2-ONE (For reference only, please check.)
IMDG: 5-METHYLHEXAN-2-ONE (For reference only, please check.)
IATA: 5-METHYLHEXAN-2-ONE (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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