

Chemical Safety Data Sheet MSDS / SDS

2,6-dimethylheptan-4-one 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: 2,6-dimethylheptan-4-one

CAS: 108-83-8

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

Specific target organ toxicity - single exposure, Category 3

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

Hazard statement(s)

H226 Flammable liquid and vapour

H335 May cause respiratory irritation

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.

P319 Get medical help if you feel unwell.

Storage

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

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P405 Store locked up.

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: 2,6-dimethylheptan-4-one

Common names and synonyms: 2,6-dimethylheptan-4-one

CAS number: 108-83-8

EC number: 203-620-1

Concentration: 100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Artificial respiration may be needed. Refer for medical attention.

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. Give a slurry of activated charcoal in water to drink. Refer for medical attention .

Most important symptoms/effects, acute and delayed

Inhalation of vapor causes irritation of nose and throat. Ingestion causes irritation of mouth and stomach. Vapor irritates eyes.

Contact with liquid irritates skin. (USCG, 1999)

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

INHALATION. Symptoms: Cough. Dizziness. Headache. Nausea. Sore throat. Vomiting. First aid: Fresh air, rest. Artificial respiration may be needed. Refer for medical attention. **SKIN:** Symptoms: Redness. Numbness. First aid: Remove contaminated clothes. Rinse and then wash skin with water and soap. **EYES:** Symptoms: Redness. Pain. First aid: First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then take to a doctor. **INGESTION:** First aid: Rinse mouth. Give a slurry of activated charcoal in water to drink. Refer for medical attention.

SECTION 5: Firefighting measures

Suitable extinguishing media

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

Specific hazards arising from the chemical

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]: **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. 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 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 particulates adapted to the airborne concentration of the substance. Ventilation. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: filter respirator for organic gases and particulates adapted to the airborne concentration of the substance. Ventilation. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

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. Ventilate area of spill or leak. Absorb liquids in vermiculite, dry sand, earth, peat, carbon, or similar material and deposit in sealed containers. 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 49°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. Separated from strong 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: 25 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 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:	Colourless.
Odour:	Peppermint odor
Melting point/freezing point:	-45.98°C. Atm. press.:Ca. 101.3 kPa.
Boiling point or initial boiling point and boiling range:	168.26°C. Atm. press.:101.3 kPa.
Flammability:	Class II Combustible Liquid: Fl.P. at or above 100°F and below 140°F.

Lower and upper explosion limit/flammability limit:	Lower flammable limit: 0.8% by volume @ 200 deg F (93 deg C); Upper flammable limit: 7.1% by volume @ 200 deg F (93 deg C)
Flash point:	49 °C. Atm. press.:Ca. 101.3 kPa.
Auto-ignition temperature:	345 °C. Atm. press.:Ca. 101.3 kPa.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	dynamic viscosity (in mPa s) = 1.05. Temperature:20°C. Remarks:Referenc: Ullmann's Encyclopedia of Industrial Chemistry,.;dynamic viscosity (in mPa s) = 0.869. Temperature:25.0°C. Remarks:Reference: Kirk-Othmer Encyclopedia of Chemical Technology.
Solubility:	Slightly soluble (NTP, 1992)
Partition coefficient n-octanol/water:	log Pow = 3.71. Temperature:25 °C. Remarks:PH not relevant for HPLC method, as the substance is not ionizable.
Vapour pressure:	0.23 kPa. Temperature:20 °C. Remarks:Reference: Ullmann.;1.7 mm Hg. Temperature:20 °C. Remarks:Reference: Verschueren/Hawley.;2.3 mm Hg. Temperature:30 °C. Remarks:Reference: Verschueren.
Density and/or relative density:	0.81 g/ml. Temperature:20 °C.;0.81 g/cm ³ . Temperature:20 °C.
Relative vapour density:	4.9 (vs air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Reacts with oxidants. Attacks some forms of plastic.

Chemical stability

no data available

Possibility of hazardous reactions

Flammable liquid when exposed to heat or flame ...DIISOBUTYL KETONE may attack some plastics. It reacts with oxidizers. (NTP, 1992)

Conditions to avoid

no data available

Incompatible materials

Reacts with oxidants. Attacks some forms of plastics.

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and fumes.

SECTION 11: Toxicological information**Acute toxicity**

Oral: LD50 - rat (male/female) - > 2 000 mg/kg bw.

Inhalation: LC50 - rat - > 14.5 mg/L air (nominal).

Dermal: LD50 - rat (male/female) - > 2 000 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. Exposure to high concentrations 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.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - *Oncorhynchus mykiss* (previous name: *Salmo gairdneri*) - 30 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - 37.2 mg/L - 48 h.

Toxicity to algae: EC50 - *Pseudokirchneriella subcapitata* (previous names: *Raphidocelis subcapitata*, *Selenastrum capricornutum*) - 46.9 mg/L - 72 h.

Toxicity to microorganisms: IC50 - aerobic microorganisms - 255 mg/L - 16 h.

Persistence and degradability

AEROBIC: Using standard BOD dilution techniques with acclimated microbial cultures, theoretical BODs of 37.4-46.7% were measured for diisobutyl ketone over 5-day incubation periods(1,2). Diisobutyl ketone had BODs of 4, 39, 57, and 88% of theoretical measured over 5, 10, 15, and 20 day incubation periods, respectively, using standard BOD dilution techniques and a non-acclimated sewage inoculum(3); theoretical BODs of 4, 9, and 18% were measured over 10, 15, and 20 day incubation periods, respectively, using a synthetic salt BOD dilution water and a non-acclimated sewage inoculum(3).

Bioaccumulative potential

An estimated BCF of 7 was calculated in fish for diisobutyl ketone(SRC), using a water solubility of 2,640 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 diisobutyl ketone is estimated as 57(SRC), using a water solubility of 2,640 mg/L(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that diisobutyl ketone is expected to have 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: UN1157 (For reference only, please check.)

IMDG: UN1157 (For reference only, please check.)

IATA: UN1157 (For reference only, please check.)

UN Proper Shipping Name

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

IMDG: DIISOBUTYL KETONE (For reference only, please check.)

IATA: DIISOBUTYL KETONE (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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