Chemical Safety Data Sheet MSDS / SDS

5-methylheptan-3-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-methylheptan-3-one

CAS: 541-85-5

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
Eye irritation, Category 2

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
H319 Causes serious eye irritation
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/...
P264 Wash ... thoroughly after handling.
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.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
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:	5-methylheptan-3-one
Common names and synonyms:	5-methylheptan-3-one
CAS number:	541-85-5
EC number:	208-793-7
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. Give one or two glasses of water to drink. Refer for medical attention .

Most important symptoms/effects, acute and delayed

no data available

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

no data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Use water spray, powder, foam, carbon dioxide.

Specific hazards arising from the chemical

Flammable. Above 43°C explosive vapour/air mixtures may be formed.

Special protective actions for fire-fighters

Use water spray, powder, foam, carbon dioxide. In case of fire: keep cylinder 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. Remove all ignition sources. 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. 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. Remove all ignition sources. 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. Do NOT wash away into sewer.

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 43°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, strong bases and strong reducing agents. Well closed.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 10 ppm as TWA.MAK: 53 mg/m3, 10 ppm; peak limitation category: I(2); pregnancy risk group: D.EU-OEL: 53 mg/m3, 10 ppm as TWA; 107 mg/m3, 20 ppm as STEL

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.

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:	Liquid.
Colour:	Colorless.
Odour:	no data available
Melting point/freezing point:	-57 °C. Remarks:Experimental conditions not reported.
Boiling point or initial boiling point and boiling range:	159 °C. Remarks:Experimental conditions not reported.
Flammability:	Class II Combustible Liquid: Fl.P. at or above 100°F and below 140°F.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	46 °C.
Auto-ignition temperature:	413 °C. Atm. press.:98 675 Pa. Remarks:Main study: Third experiment.;409 °C. Atm. press.:99 423 Pa. Remarks:Main study: Second experiment.;411 °C. Atm. press.:99 476 Pa. Remarks:Main study: First experiment.
Decomposition temperature:	no data available
pH:	no data available

Kinematic viscosity:	0.848. Temperature:20°C. Remarks:Standard deviation 0.004 mPa s.
Solubility:	in water, g/100ml at 20°C: 0.3
Partition coefficient n-octanol/water:	log Pow = 1.98. Temperature:25 °C. Remarks:PH not reported.
Vapour pressure:	270 Pa. Temperature:25 °C.
Density and/or relative density:	0.822 g/cm3. Temperature:20 °C.
Relative vapour density:	(air = 1): 4.4
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Reacts with oxidants, strong reducing agents and strong bases. This generates fire hazard.

Chemical stability

no data available

Possibility of hazardous reactions

The vapour is heavier than air and may travel along the ground; distant ignition possible.

Conditions to avoid

no data available

Incompatible materials

Strong oxidizers

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

Oral: approximate LD50 - rat (male) - 2 760 mg/kg bw.

Inhalation: LC0 - rat (male) - 9.4 mg/L air.

Dermal: approximate LD50 - rabbit (male) - > 20 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 central nervous system.

Exposure far above the OEL could cause unconsciousness.

STOT-repeated exposure

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

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 - Carassius auratus - 80 mg/L - 24 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 517 mg/L - 24 h.

Toxicity to algae: TT - Microcystis aeruginosa - 40 mg/L - 8 d.

Toxicity to microorganisms: TT - Pseudomonas putida - 25 mg/L - 16 h.

Persistence and degradability

no data available

Bioaccumulative potential

no data available

Mobility in soil

no data available

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: UN2271 (For reference only, please check.)
IMDG: UN2271 (For reference only, please check.)
IATA: UN2271 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: ETHYL AMYL KETONE (For reference only, please check.)
IMDG: ETHYL AMYL KETONE (For reference only, please check.)
IATA: ETHYL AMYL 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

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/

Other Information

Explosive limits are unknown in literature, although the substance is flammable and has a flash point <61°C. The odour warning when the exposure limit value is exceeded is insufficient.