Chemical Safety Data Sheet MSDS / SDS

Pentan-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: Pentan-3-one

CAS: 96-22-0

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 2
Specific target organ toxicity - single exposure, Category 3

Specific target organ toxicity – single exposure, Category 3

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H225 Highly flammable liquid and vapour
H335 May cause respiratory irritation
H336 May cause drowsiness or dizziness

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:	Pentan-3-one
Common names and synonyms:	Pentan-3-one
CAS number:	96-22-0
EC number:	202-490-3
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.

Most important symptoms/effects, acute and delayed

Liquid causes eye burn. Vapor irritates eyes, nose and throat; can cause headache, dizziness, nausea, weakness, and loss of consciousness. (USCG, 1999)

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

INHALATION. Symptoms: Cough. Shortness of breath. First aid: Fresh air, rest. Refer for medical attention. SKIN: Symptoms: Dry skin. Redness. First aid: Remove contaminated clothes. Rinse skin with plenty of water or shower. 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: First aid: Rinse mouth.

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 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 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 and spilled liquid in sealable metal (mild steel) 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. Collect leaking and spilled liquid in sealable metal (mild steel) 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

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 comfined 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. Closed system, ventilation, explosion-proof electrical equipment and lighting. Do NOT use compressed air for filling, discharging, or 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

Fireproof. Separated from oxidants.Diethyl ketone must be stored to avoid contact with oxidizing materials (such as peroxides, perchlorates, chlorates, permanganates, and nitrates) Since violent reactions may occur. Store in tightly closed containers in a cool, well ventilated area away from sources of heat. Sources of ignition such as smoking and open flames are prohibited where diethyl ketone is handled, used or stored in a manner that could create a potential fire or explosion hazard. Metal containers involving the transfer of 5 gallons or more of diethyl ketone should be grounded and bonded. Drums must be equipped with self-closing valves, pressure vacuum bungs, and flame arresters. Use only non-sparking tools and equipment, especially when opening and closing containers of diethyl ketone. Wherever this diethyl ketone is used, handled, manufactured, or stored, use explosion-proof electrical equipment and fittings.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 200 ppm as TWA; 300 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.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Diethyl ketone is a clear colorless liquid with an acetone-like odor. Flash point 55°F. Less dense than water. Vapors heavier than air.
Colour:	Colorless, mobile liquid
Odour:	Acetone odor
Melting point/freezing point:	357°C(lit.)

Boiling point or initial boiling point and boiling range:	101.5°C(lit.)
Flammability:	Class IB Flammable Liquid: Fl.P. below 73°F and BP at or above 100°F.
Lower and upper explosion limit/flammability limit:	Lower flammable limit: 1.6% by volume; Upper flammable limit: 6.4% by volume
Flash point:	7°C
Auto-ignition temperature:	845°F
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	0.444 mPa s at 25 deg C
Solubility:	5 % (NIOSH, 2016)
Partition coefficient n-octanol/water:	log Kow = 0.99
Vapour pressure:	20 mm Hg (28 °C)
Density and/or relative density:	0.813g/mLat 25°C(lit.)
Relative vapour density:	3 (vs air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Reacts violently with oxidants. This generates fire and explosion hazard. Attacks many plastics.

Chemical stability

no data available

Possibility of hazardous reactions

Dangerous fire hazard when exposed to heat or flame ...The vapour is heavier than air and may travel along the ground; distant ignition possible. The vapour mixes well with air, explosive mixtures are easily formed.DIETHYL KETONE is incompatible with the following: Strong oxidizers, alkalis, mineral acids, (hydrogen peroxide + nitric acid) (NIOSH, 2016).

Conditions to avoid

no data available

Incompatible materials

Violent reaction with oxidizers, causing fire and explosion hazard. Forms explosive mixture with air. Incompatible with strong acids, aliphatic amines. Attacks many plastics, rubber and coatings. May accumulate static electrical charges, and may cause ignition of its vapors.

Hazardous decomposition products

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

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Rat oral 2.14 g/kg

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

The substance is irritating to the eyes, skin and respiratory tract.

STOT-repeated exposure

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

Aspiration hazard

A harmful contamination of the air can be reached rather quickly on evaporation of this substance at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 Pimephales promelas (fathead minnow) 27-28 days old 1540 mg/L/96 hr (confidence limit: 1470-1600 mg/L) at 24.2 deg C (hardness 46.2 mg/L calcium carbonate, pH 7.88) /Purity 98%; Conditions of bioassay not specified

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: LC50 Scenedesmus subspicatus (algae) = >500 mg/L/72 hours /Conditions of bioassay not specified

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: Several investigators have shown that diethyl ketone readily biodegrades in screening tests using sewage or sludge(1-5). Using a standard BOD dilution technique and acclimated sewage inocula, a BOD of 66.4%(1) and 89%(2) of theoretical was observed over a 5 day incubation period. Using a standard BOD dilution technique and unacclimated sewage inocula, BOD values of 50.8%(3) and 38%(4) of theoretical was observed over a 10 day incubation period. The percent theoretical BOD of diethyl ketone in a semi-continuous activated sludge (SCAS) biological treatment simulation test was 38% over a 24 hour incubation period(5).

Bioaccumulative potential

An estimated BCF of 3 was calculated in fish for diethyl ketone(SRC), using a log Kow of 0.99(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 diethyl ketone is estimated as 82(SRC), using a log Kow of 0.99(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that diethyl 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: UN1156 (For reference only, please check.)
IMDG: UN1156 (For reference only, please check.)
IATA: UN1156 (For reference only, please check.)

UN Proper Shipping Name

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