

## Chemical Safety Data Sheet MSDS / SDS

## Octan-3-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: Octan-3-one

CAS: 106-68-3

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

Relevant identified uses: For R&amp;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 3

Skin irritation, Category 2

## GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

### Hazard statement(s)

H226 Flammable liquid and vapour

H315 Causes skin 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.

#### 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.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P321 Specific treatment (see ... on this label).

P332+P317 If skin irritation occurs: Get medical help.

P362+P364 Take off contaminated clothing and wash it before reuse.

#### 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:	Octan-3-one
Common names and synonyms:	Octan-3-one
CAS number:	106-68-3
EC number:	203-423-0
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

May be harmful by inhalation, ingestion or skin absorption. Vapor or mist is irritating to eyes, mucous membrane and upper respiratory tract. Causes skin irritation. (USCG, 1999)

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

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Ketones and related compounds

## **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 spread fire. 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.

### **Specific hazards arising from the chemical**

Special Hazards of Combustion Products: Vapor may travel considerable distance to a source of ignition and flash back. (USCG, 1999)

### **Special protective actions for fire-fighters**

Wear self-contained breathing apparatus for firefighting if necessary.

## **SECTION 6: Accidental release measures**

### **Personal precautions, protective equipment and emergency procedures**

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

### **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

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

Component	Octan-3-one			
CAS No.	106-68-3			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m <sup>3</sup>	ppm	mg/m <sup>3</sup>
Austria	25	130	50	260
	Remarks			

### 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 tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

### Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

### Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

### Thermal hazards

no data available

## SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Ethyl amyl ketone is a clear colorless liquid with a pungent odor. Insoluble in water and partially soluble in alcohol. Flash point of 138°F. Vapors are denser than air and may have a narcotic effect in high concentrations. Used in making perfumes and as a solvent for nitrocellulose and vinyl resins.
Colour:	Colorless liquid
Odour:	Mild fruity odor
Melting point/freezing point:	265°C(lit.)
Boiling point or initial boiling point and boiling range:	167°C
Flammability:	Flammable.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	54°C(lit.)

Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	Insoluble (NIOSH, 2016)
Partition coefficient n-octanol/water:	log Kow = 2.22 (est)
Vapour pressure:	1.5mmHg at 25°C
Density and/or relative density:	0.822
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

**FIRE HAZARD: MODERATE.** The vapour is heavier than air and may travel along the ground; distant ignition possible. Ketones, such as ETHYL AMYL KETONE, are reactive with many acids and bases liberating heat and flammable gases (e.g., H<sub>2</sub>). 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 (H<sub>2</sub>) and heat. Ketones are incompatible with isocyanates, aldehydes, cyanides,

peroxides, and anhydrides. They react violently with aldehydes, HNO<sub>3</sub>, HNO<sub>3</sub> + H<sub>2</sub>O<sub>2</sub>, and HClO<sub>4</sub>.

**Conditions to avoid**

no data available

**Incompatible materials**

Strong oxidizers

**Hazardous decomposition products**

no data available

**SECTION 11: Toxicological information**

**Acute toxicity**

Oral: LD<sub>50</sub> Rat oral >5 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**

no data available

**STOT-repeated exposure**

no data available

**Aspiration hazard**

no data available

**SECTION 12: Ecological information****Toxicity**

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: LC50; Species: Daphnia magna (Water flea, age < or =24 hr); Conditions: freshwater, static, 20-22 deg C, pH 7.6-7.7, hardness 16 dH; Concentration: 517 mg/L for 24 hr

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

**Persistence and degradability**

AEROBIC: 3-Octanone, at 500 mg/L, was inoculated with activated sludge from Columbus (municipal treatment plant) and Brookside (residential waste); BOD reached an average 1.1, 2.0, and 3.4% of the theoretical oxygen demand within 6, 12, and 24 hours, respectively(1). Columbus sludge had a greater ability to oxidize this compound, reaching 150 mg/L BOD within 24 hours(1).

**Bioaccumulative potential**

An estimated BCF of 7 was calculated in fish for 3-octanone(SRC), using a water solubility of 2600 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 3-octanone is estimated as 58(SRC), using a water solubility of 2600 mg/L(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that 3-octanone 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: 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**

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](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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