

## Chemical Safety Data Sheet MSDS / SDS

## Heptanal 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: Heptanal  
CAS: 111-71-7

**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  
Skin irritation, Category 2

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3

### GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

### Hazard statement(s)

H226 Flammable liquid and vapour

H315 Causes skin irritation

H412 Harmful to aquatic life with long lasting effects

### 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.

P273 Avoid release to the environment.

### 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: Heptanal

Common names and synonyms: Heptanal

CAS number: 111-71-7

EC number: 203-898-4

Concentration: 100%

**SECTION 4: First aid measures**

**Description of necessary first-aid measures**

**If inhaled**

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

**Following skin contact**

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

**Following eye contact**

Rinse with pure water for at least 15 minutes. Consult a doctor.

**Following ingestion**

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

### **Most important symptoms/effects, acute and delayed**

Excerpt from ERG Guide 129 [Flammable Liquids (Water-Miscible / Noxious)]: May cause toxic effects if inhaled or absorbed through skin. Inhalation or contact with material may irritate or burn skin and eyes. Fire will produce irritating, corrosive and/or toxic gases. Vapors may cause dizziness or suffocation. Runoff from fire control or dilution water may cause pollution. (ERG, 2016)

### **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. Aldehydes and Related Compounds

## **SECTION 5: Firefighting measures**

### **Suitable extinguishing media**

Excerpt from ERG Guide 129 [Flammable Liquids (Water-Miscible / Noxious)]: CAUTION: All these products have a very low flash point: Use of water spray when fighting fire may be inefficient. SMALL FIRE: Dry chemical, CO<sub>2</sub>, water spray or alcohol-resistant foam. Do not use dry chemical extinguishers to control fires involving nitromethane (UN1261) or nitroethane (UN2842). LARGE FIRE: Water spray, fog or alcohol-resistant foam. Do not use straight streams. Move containers from fire area if you can do it without risk. FIRE INVOLVING TANKS OR CAR/TRAILER LOADS: Fight fire from maximum distance or use unmanned hose holders or monitor nozzles. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks engulfed in fire. For massive fire, use unmanned hose holders or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2016)

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

Excerpt from ERG Guide 129 [Flammable Liquids (Water-Miscible / Noxious)]: 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**

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

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

### 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

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

## SECTION 8: Exposure controls/personal protection

### Control parameters

### Occupational Exposure limit values

no data available

### 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/flare 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:	N-heptaldehyde is a colorless, oily liquid with a penetrating fruity odor. Insoluble in water and less dense than water. Hence floats on water. Flash point near 141°F. Used to make perfumes and pharmaceuticals.
Colour:	Oily colorless liquid
Odour:	FATTY, PUNGENT ODOR
Melting point/freezing point:	413°C(lit.)

Boiling point or initial boiling point and boiling range:	155°C
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	34°C(lit.)
Auto-ignition temperature:	Autoflammability: 250 deg C at 1013 hPa
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	0.977 cP at 15 deg C; 0.791 cP at 30 deg C
Solubility:	less than 1 mg/mL at 70° F (NTP, 1992)
Partition coefficient n-octanol/water:	log Kow = 2.29 (est)
Vapour pressure:	3.85mmHg at 25°C
Density and/or relative density:	0.817
Relative vapour density:	3.9 (NTP, 1992) (Relative to Air)
Particle characteristics:	no data available

## SECTION 10: Stability and reactivity

### Reactivity

Flammable. Insoluble in water.

### **Chemical stability**

no data available

### **Possibility of hazardous reactions**

Flammable/combustible material; may be ignited by heat, sparks or flames. N-HEPTALDEHYDE may undergo exothermic self-condensation or polymerization reactions in the presence of acids. May generate flammable and/or toxic gases with azo, diazo compounds, dithiocarbamates, nitrides, and strong reducing agents. Is readily oxidized to give heptanoic acid. Can react with air to give first peroxy acids, and ultimately heptanoic acid. These autoxidation reactions are activated by light, catalyzed by salts of transition metals, and are autocatalytic (catalyzed by the products of the reaction). The presence of stabilizers (antioxidants) retards autoxidation. Incompatible with strong oxidizers, bases and reducing agents. (NTP, 1992)

### **Conditions to avoid**

no data available

### **Incompatible materials**

no data available

### **Hazardous decomposition products**

no data available

## **SECTION 11: Toxicological information**

### **Acute toxicity**

Oral: LD50 Rat oral 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**

no data available

**STOT-repeated exposure**

no data available

**Aspiration hazard**

no data available

**SECTION 12: Ecological information**

**Toxicity**

Toxicity to fish: LC50; Species: Pimephales promelas (Fathead minnow, 26-34 day old juvenile); Conditions: freshwater, continuous flow through system; Concentration: 37.9 mg/L for 96 hr /metabolic precursor, 1-heptanol

Toxicity to daphnia and other aquatic invertebrates: EC50; Species: Daphnia magna (Water flea); Conditions: freshwater, static, 19-21 deg C, pH 7.8-8.2, dissolved oxygen 9.1 + or -0.1 mg/L, water hardness 190-230 mg/L CaCO3; Concentration: >200 mg/L for 24 hr; Effect: immobilization /98% (methyl hexanoate, 1%)

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

### **Persistence and degradability**

AEROBIC: n-Heptanal biodegraded fast with acclimation in a respiratory screening test using an activated sludge inoculum; using a n-heptanal concentration of 500 mg/L at 20 deg C, 14.7% of the theoretical oxygen demand was consumed in 1 day(1). In a biological treatment simulation with a continuous feed, 71% removal was achieved(2). In a groundwater recharge project in Palo Alto, CA, 70% of theoretical COD was removed(3).

### **Bioaccumulative potential**

An estimated BCF of 11 was calculated in fish for n-heptanal(SRC), using a water solubility of 1,250 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 n-heptanal is estimated as 86(SRC), using a water solubility of 1250 mg/L(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that n-heptanal 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: UN3056 (For reference only, please check.)

IMDG: UN3056 (For reference only, please check.)

IATA: UN3056 (For reference only, please check.)

### UN Proper Shipping Name

ADR/RID: n-HEPTALDEHYDE (For reference only, please check.)

IMDG: n-HEPTALDEHYDE (For reference only, please check.)

IATA: n-HEPTALDEHYDE (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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