

SAFETY DATA SHEETS

According to the UN GHS revision 10

Version: 1.0
Creation Date: July 15, 2024
Revision Date: July 15, 2024

SECTION 1: Identification

<!--{productinfo}-->

1.3 Recommended use of the chemical and restrictions on use

Identified uses	Industrial and scientific research use.
Uses advised against	no data available

1.4 Supplier's details

<!--{companyinfo}-->

1.5 Emergency phone number

<!--{Emergency phone number}-->

SECTION 2: Hazard identification

2.1 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

2.2 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)	P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
Prevention	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/...
Response	P264 Wash ... thoroughly after handling. P273 Avoid release to the environment. 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.

2.3 Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
Heptanal	Heptanal	111-71-7	203-898-4	≈ 99%

SECTION 4: First-aid measures

4.1 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.

4.2 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)

4.3 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: Fire-fighting measures

5.1 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, CO₂, 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)

5.2 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)

5.3 Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

6.1 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.

6.2 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.

6.3 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

7.1 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.

7.2 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

8.1 Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

8.2 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.

8.3 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

10.1 Reactivity

Flammable. Insoluble in water.

10.2 Chemical stability

no data available

10.3 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)

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

no data available

10.6 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

12.1 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

12.2 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).

12.3 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).

12.4 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.

12.5 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 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

14.1 UN Number

ADR/RID: UN3056 (For reference only, please check.)

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

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

14.2 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.)

14.3 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.)

14.4 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.)

14.5 Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
Heptanal	Heptanal	111-71-7	203-898-4
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.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Listed.
Korea Existing Chemicals List (KECL)			Listed.

SECTION 16: Other information

Information on revision

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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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