

SAFETY DATA SHEET

Version 5.6
Revision Date 04/21/2017
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1. PRODUCT AND COMPANY IDENTIFICATION**1.1 Product identifiers**

Product name : Heptanal

Product Number : W254002

Brand : Aldrich

CAS-No. : 111-71-7

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 3), H226

Skin irritation (Category 2), H315

Acute aquatic toxicity (Category 2), H401

Chronic aquatic toxicity (Category 3), H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word

Warning

Hazard statement(s)

H226

Flammable liquid and vapour.

H315

Causes skin irritation.

H401

Toxic to aquatic life.

H412

Harmful to aquatic life with long lasting effects.

Precautionary statement(s)

P210

Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P233

Keep container tightly closed.

P240

Ground/bond container and receiving equipment.

P241

Use explosion-proof electrical/ ventilating/ lighting/ equipment.

P242

Use only non-sparking tools.

P243

Take precautionary measures against static discharge.

P264	Wash skin thoroughly after handling.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P235	Store in a well-ventilated place. Keep cool.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : Heptaldehyde
Enanthaldehyde
Oenanthaldehyde
1-Heptanal
Aldehyde C7

Formula : C₇H₁₄O
Molecular weight : 114.19 g/mol
CAS-No. : 111-71-7
EC-No. : 203-898-4

Hazardous components

Component	Classification	Concentration
Heptanal		
	Flam. Liq. 3; Skin Irrit. 2; Aquatic Acute 2; Aquatic Chronic 3; H226, H315, H401, H412	90 - 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

- 4.3 Indication of any immediate medical attention and special treatment needed**
No data available

5. FIREFIGHTING MEASURES

- 5.1 Extinguishing media**
Suitable extinguishing media
Dry powder Dry sand
Unsuitable extinguishing media
Do NOT use water jet.
- 5.2 Special hazards arising from the substance or mixture**
No data available
- 5.3 Advice for firefighters**
Wear self-contained breathing apparatus for firefighting if necessary.
- 5.4 Further information**
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

- 6.1 Personal precautions, protective equipment and emergency procedures**
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.
For personal protection see section 8.
- 6.2 Environmental precautions**
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.
- 6.3 Methods and materials for containment and cleaning up**
Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).
- 6.4 Reference to other sections**
For disposal see section 13.

7. HANDLING AND STORAGE

- 7.1 Precautions for safe handling**
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.
For precautions see section 2.2.
- 7.2 Conditions for safe storage, including any incompatibilities**
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Handle and store under inert gas.
- 7.3 Specific end use(s)**
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

- 8.1 Control parameters**
Components with workplace control parameters
Contains no substances with occupational exposure limit values.
Hazardous components without workplace control parameters
- 8.2 Exposure controls**
Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Splash contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: 120 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Impervious clothing, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

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

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- | | |
|---|--|
| a) Appearance | Form: clear, liquid
Colour: light yellow |
| b) Odour | No data available |
| c) Odour Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/range: -43 °C (-45 °F) - lit. |
| f) Initial boiling point and boiling range | 153 °C (307 °F) - lit. |
| g) Flash point | 35 °C (95 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 5.2 %(V)
Lower explosion limit: 1.1 %(V) |
| k) Vapour pressure | 6.6 hPa (5.0 mmHg) at 25 °C (77 °F)
5.0 hPa (3.8 mmHg) at 20 °C (68 °F) |
| l) Vapour density | No data available |

m) Relative density	0.817 g/cm ³ at 25 °C (77 °F)
n) Water solubility	slightly soluble
o) Partition coefficient: n-octanol/water	log Pow: 2.8 at 20 °C (68 °F)
p) Auto-ignition temperature	205 °C (401 °F) at 990 hPa (743 mmHg)
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

Vapours may form explosive mixture with air.

10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

Oxidizing agents, Strong bases, Strong reducing agents

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - > 5,000 mg/kg

(OECD Test Guideline 401)

LD50 Dermal - Rabbit - > 5,000 mg/kg

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Skin irritation

(OECD Test Guideline 404)

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

Maximisation Test - Guinea pig

Result: Not a skin sensitizer.

(OECD Test Guideline 406)

Germ cell mutagenicity

No data available

reverse mutation assay
Salmonella typhimurium
Result: negative

In vitro mammalian cell gene mutation test
mouse lymphoma cells
Result: negative

Chromosome aberration test in vitro
Human lymphocytes
Result: negative

Carcinogenicity

No data available

- IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
- NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
- OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

Repeated dose toxicity Rat - Oral - OECD Test Guideline 408
RTECS: MI6900000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

No data available

- | | |
|---|--|
| Toxicity to fish | semi-static test LC50 - Oncorhynchus mykiss (rainbow trout) - 12 mg/l - 96 h (OECD Test Guideline 203) |
| Toxicity to daphnia and other aquatic invertebrates | flow-through test EC50 - Daphnia magna (Water flea) - 4.13 mg/l - 48 h (OECD Test Guideline 202) |
| Toxicity to algae | static test EC50 - Pseudokirchneriella subcapitata - 2.9 mg/l - 72 h (OECD Test Guideline 201) |
| Toxicity to bacteria | EC50 - Pseudomonas putida - 580 mg/l - 3 h (OECD Test Guideline 209) |

12.2 Persistence and degradability

Biodegradability Result: 63 - 74 % - Readily biodegradable.
(OECD Test Guideline 301D)

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Toxic to aquatic life.

13. DISPOSAL CONSIDERATIONS**13.1 Waste treatment methods****Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION**DOT (US)**

UN number: 3056 Class: 3 Packing group: III

Proper shipping name: n-Heptaldehyde

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

IMDG

UN number: 3056 Class: 3 Packing group: III EMS-No: F-E, S-D

Proper shipping name: n-HEPTALDEHYDE

Marine pollutant:yes

IATA

UN number: 3056 Class: 3 Packing group: III

Proper shipping name: n-Heptaldehyde

15. REGULATORY INFORMATION**SARA 302 Components**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Heptanal	111-71-7	1989-12-01

	CAS-No.	Revision Date
Heptanal	111-71-7	1989-12-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Heptanal	111-71-7	1989-12-01

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Flam. Liq.	Flammable liquids
H226	Flammable liquid and vapour.
H315	Causes skin irritation.
H401	Toxic to aquatic life.
H412	Harmful to aquatic life with long lasting effects.
Skin Irrit.	Skin irritation

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	
Flammability:	3
Physical Hazard	0

NFPA Rating

Health hazard:	2
Fire Hazard:	3
Reactivity Hazard:	0

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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