

MATERIAL SAFETY DATA SHEET

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Version 1.4

Section 1 - Product and Company Information

Product Name HEPTALDEHYDE, 95%
Product Number H2120
Brand SIAL

Company Sigma-Aldrich
Address 3050 Spruce Street
SAINT LOUIS MO 63103 US

Technical Phone: 800-325-5832
Fax: 800-325-5052
Emergency Phone: 314-776-6555

Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313
1-HEPTALDEHYDE, STAB.	111-71-7	No

Formula C7H14O
Synonyms Enanthal * Enanthaldehyde * Enanthole *
Heptaldehyde * Heptyl aldehyde * Oenanthal *
Oenanthaldehyde * Oenanthic aldehyde * Oenanthol

RTECS Number: MI6900000

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Flammable. Irritant.

Irritating to eyes, respiratory system and skin.

HMIS RATING

HEALTH: 2

FLAMMABILITY: 3

REACTIVITY: 0

NFPA RATING

HEALTH: 2

FLAMMABILITY: 3

REACTIVITY: 0

For additional information on toxicity, please refer to Section 11.

Section 4 - First Aid Measures

ORAL EXPOSURE

If swallowed, wash out mouth with water provided person is conscious. Call a physician.

INHALATION EXPOSURE

If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

DERMAL EXPOSURE

In case of contact, immediately wash skin with soap and copious amounts of water.

EYE EXPOSURE

In case of contact, immediately flush eyes with copious amounts of water for at least 15 minutes.

Section 5 - Fire Fighting Measures

FLAMMABLE HAZARDS

Flammable Hazards: Yes

EXPLOSION HAZARDS

Vapor may travel considerable distance to source of ignition and flash back. Container explosion may occur under fire conditions.

FLASH POINT

95 °F 35 °C Method: closed cup

EXPLOSION LIMITS

Lower: 1.1 % Upper: 5.2 %

AUTOIGNITION TEMP

N/A

FLAMMABILITY

N/A

EXTINGUISHING MEDIA

Suitable: For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

FIREFIGHTING

Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.
Specific Hazard(s): Flammable liquid. Emits toxic fumes under fire conditions.

Section 6 - Accidental Release Measures

PROCEDURE TO BE FOLLOWED IN CASE OF LEAK OR SPILL

Evacuate area. Shut off all sources of ignition. Use nonsparking tools.

PROCEDURE(S) OF PERSONAL PRECAUTION(S)

Wear self-contained breathing apparatus, rubber boots, and heavy rubber gloves.

METHODS FOR CLEANING UP

Cover with dry-lime, sand, or soda ash. Place in covered containers using non-sparking tools and transport outdoors. Ventilate area and wash spill site after material pickup is complete.

Section 7 - Handling and Storage

HANDLING

User Exposure: Do not breathe vapor. Do not get in eyes, on

skin, on clothing. Avoid prolonged or repeated exposure.

STORAGE

Suitable: Keep tightly closed. Keep away from heat, sparks, and open flame.

SPECIAL REQUIREMENTS

Handle and store under inert gas.

Section 8 - Exposure Controls / PPE

ENGINEERING CONTROLS

Safety shower and eye bath. Use nonsparking tools. Mechanical exhaust required.

PERSONAL PROTECTIVE EQUIPMENT

Respiratory: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). 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.
Hand: Compatible chemical-resistant gloves.
Eye: Chemical safety goggles.

GENERAL HYGIENE MEASURES

Remove and wash contaminated clothing promptly. Wash thoroughly after handling.

Section 9 - Physical/Chemical Properties

Appearance	Color: Very faintly yellow-green Form: Clear liquid	
Property	Value	At Temperature or Pressure
Molecular Weight	114.19 AMU	
pH	N/A	
BP/BP Range	40.0 - 42.0 °C	11 mmHg
MP/MP Range	- 43.0 °C	
Freezing Point	N/A	
Vapor Pressure	N/A	
Vapor Density	N/A	
Saturated Vapor Conc.	N/A	
SG/Density	0.818 g/cm ³	
Bulk Density	N/A	
Odor Threshold	N/A	
Volatile%	N/A	
VOC Content	N/A	
Water Content	N/A	
Solvent Content	N/A	
Evaporation Rate	N/A	
Viscosity	N/A	
Surface Tension	N/A	
Partition Coefficient	N/A	
Decomposition Temp.	N/A	
Flash Point	95 °F 35 °C	Method: closed cup
Explosion Limits	Lower: 1.1 % Upper: 5.2 %	
Flammability	N/A	
Autoignition Temp	N/A	

Refractive Index 1.413
Optical Rotation N/A
Miscellaneous Data N/A
Solubility Solubility in Water:Slightly.
Other Solvents: ETHANOL, DIETHYLETHER, DMSO

N/A = not available

Section 10 - Stability and Reactivity

STABILITY

Stable: Stable.
Conditions of Instability: Light.
Materials to Avoid: Oxidizing agents, Strong bases, Strong reducing agents.

HAZARDOUS DECOMPOSITION PRODUCTS

Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide.

HAZARDOUS POLYMERIZATION

Hazardous Polymerization: Will not occur

Section 11 - Toxicological Information

ROUTE OF EXPOSURE

Skin Contact: Causes skin irritation.
Skin Absorption: May be harmful if absorbed through the skin.
Eye Contact: Causes eye irritation.
Inhalation: May be harmful if inhaled. Material is irritating to mucous membranes and upper respiratory tract.
Ingestion: May be harmful if swallowed.

TOXICITY DATA

Oral
Rat
3200 mg/kg
LD50
Remarks: Behavioral:Muscle weakness.

Inhalation
Rat
> 18,400 mg/m3
LC50
Remarks: Behavioral:Excitement. Lungs, Thorax, or Respiration:Respiratory stimulation. Gastrointestinal:Changes in structure or function of salivary glands.

Intraperitoneal
Rat
1600 MG/KG
LD50
Remarks: Gastrointestinal:Hypermotility, diarrhea.
Behavioral:Muscle weakness.

Oral
Mouse
3200 mg/kg
LD50
Remarks: Behavioral:Muscle weakness.

Intraperitoneal

Mouse
400 MG/KG
LD50
Remarks: Behavioral:Somnolence (general depressed activity).
Behavioral:Muscle weakness. Skin and Appendages: Other: Hair.

Skin
Rabbit
> 5000 mg/kg
LD50

IRRITATION DATA

Eyes
Rabbit
0.1 ml
Remarks: Severe irritation effect

Section 12 - Ecological Information

No data available.

Section 13 - Disposal Considerations

APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

Contact a licensed professional waste disposal service to dispose of this material. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Observe all federal, state, and local environmental regulations.

Section 14 - Transport Information

DOT

Proper Shipping Name: n-Heptaldehyde
UN#: 3056
Class: 3
Packing Group: Packing Group III
Hazard Label: Flammable liquid
PIH: Not PIH

IATA

Proper Shipping Name: n-Heptaldehyde
IATA UN Number: 3056
Hazard Class: 3
Packing Group: III

Section 15 - Regulatory Information

EU ADDITIONAL CLASSIFICATION

Symbol of Danger: Xi
Indication of Danger: Irritant.
R: 10-36/37/38
Risk Statements: Flammable. Irritating to eyes, respiratory system and skin.
S: 26-36
Safety Statements: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing.

US CLASSIFICATION AND LABEL TEXT

Indication of Danger: Flammable. Irritant.

Risk Statements: Irritating to eyes, respiratory system and skin.
Safety Statements: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing.

UNITED STATES REGULATORY INFORMATION

SARA LISTED: No

TSCA INVENTORY ITEM: Yes

CANADA REGULATORY INFORMATION

WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.

DSL: Yes

NDSL: No

Section 16 - Other Information

DISCLAIMER

For R&D use only. Not for drug, household or other uses.

WARRANTY

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale. Copyright 2008 Sigma-Aldrich Co. License granted to make unlimited paper copies for internal use only.