



MATERIAL SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Date of issue: 02/04/2013

Version 1.0

SECTION 1. Identification

Product identifier

Product number	806918
Product name	Heptanal (stabilised) for synthesis

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

Identified uses	Chemical for synthesis
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Details of the supplier of the safety data sheet

Company	EMD Millipore Corporation 290 Concord Road, Billerica, MA 01821, United States of America SDS Phone Support: +1-978-715-1335 General Inquiries: +1-978-715-4321 Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5) e-mail: mm_sds@merckgroup.com
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Emergency telephone	800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week
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SECTION 2. Hazards identification

GHS Classification

Flammable liquid, Category 3, H226
Carcinogenicity, Category 2, H351
Germ cell mutagenicity, Category 2, H341
Skin sensitization, Category 1, H317

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

GHS-Labeling

Hazard pictograms



Signal Word
Warning

Hazard Statements
H226 Flammable liquid and vapor.

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H317 May cause an allergic skin reaction.
H341 Suspected of causing genetic defects.
H351 Suspected of causing cancer.

Precautionary Statements

P210 Keep away from heat.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

OSHA Hazards

This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).

Other hazards

None known.

SECTION 3. Composition/information on ingredients

Formula	CH ₃ (CH ₂) ₅ CHO	C ₇ H ₁₄ O (Hill)
CAS-No.	111-71-7	
Molar mass	114.19 g/mol	

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.

n-heptanal (>= 90 % - <= 100 %)

111-71-7

hydroquinone (>= 1 % - < 5 %)

123-31-9

SECTION 4. First aid measures

Description of first-aid measures

Inhalation

After inhalation: fresh air. Consult a physician.

Skin contact

After skin contact: wash off with plenty of water. Remove contaminated clothing. Get medical attention.

Eye contact

After eye contact: rinse out with plenty of water.

Ingestion

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

irritant effects, Allergic reactions, Cough, Shortness of breath

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Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂), Foam, Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

Special hazards arising from the substance or mixture

Combustible material, Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapors possible in the event of fire.

Forms explosive mixtures with air at elevated temperatures.

Advice for firefighters

Special protective equipment for fire-fighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information

Cool closed containers exposed to fire with water spray. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid substance contact. Do not breathe vapors, aerosols. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

Environmental precautions

Do not empty into drains. Risk of explosion.

Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7 and 10).

Take up with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

SECTION 7. Handling and storage

Precautions for safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapors/aerosols.

Observe label precautions.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

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Conditions for safe storage, including any incompatibilities

Keep away from heat and sources of ignition. Keep container tightly closed in a dry and well-ventilated place.

Store at +15°C to +25°C (+59°F to +77°F).

SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Ingredients

Basis	Value	Threshold limits	Remarks
<i>hydroquinone</i> 123-31-9			
ACGIH	Time Weighted Average (TWA):	1 mg/m ³	
NIOSH/GUIDE	Ceiling Limit Value and Time Period (if specified):	2 mg/m ³	Ceiling Limit Value 15-min
OSHA_TRANS	PEL:	2 mg/m ³	
Z1A	Time Weighted Average (TWA):	2 mg/m ³	

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures

Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance.

Eye/face protection

Safety glasses

Hand protection

Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Other protective equipment:

Flame retardant antistatic protective clothing

Respiratory protection

required when vapors/aerosols are generated.

Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

SECTION 9. Physical and chemical properties

Physical state liquid

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Color	colorless
Odor	unpleasant
Odor Threshold	No information available.
pH	No information available.
Melting point	-42 °C
Boiling point/boiling range	302 °F (150 °C) at 1,013 hPa
Flash point	118 °F (48 °C) Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1.1 %(V)
Upper explosion limit	5.2 %(V)
Vapor pressure	3 hPa at 68 °F (20 °C) 11 hPa at 104 °F (40 °C)
Relative vapor density	3.93
Relative density	0.82 g/cm ³ at 68 °F (20 °C)
Water solubility	1.25 g/l at 77 °F (25 °C)
Partition coefficient: n-octanol/water	log Pow: 2.8 (IUCLID) Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	No information available.
Ignition temperature	482 °F (250 °C)

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SECTION 10. Stability and reactivity

Reactivity

Vapor/air-mixtures are explosive at intense warming.

Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Stabilizer

hydroquinone

Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents, Strong bases, strong reducing agents

Conditions to avoid

Heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

Incompatible materials

no information available

Hazardous decomposition products

no information available

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure

Inhalation, Eye contact, Skin contact

Target Organs

Eyes

Skin

Respiratory system

Central nervous system

Acute oral toxicity

LD50 rat: > 5,000 mg/kg (RTECS)

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Acute inhalation toxicity

Symptoms: Possible damages:, mucosal irritations

Acute dermal toxicity

LD50 rabbit: > 5,000 mg/kg
(RTECS)

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Eye irritation

rabbit

Result: slight irritation

OECD Test Guideline 405

Sensitization

May cause an allergic skin reaction.

Genotoxicity in vitro

Ames test

Salmonella typhimurium

Result: negative

(National Toxicology Program)

Mutagenicity (mammal cell test):

Result: negative

(IUCLID)

CMR effects

Carcinogenicity:

Suspected of causing cancer.

Mutagenicity:

Suspected of causing genetic defects.

Specific target organ systemic toxicity - single exposure

The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ systemic toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

Regarding the available data the classification criteria are not fulfilled.

Carcinogenicity

IARC	No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
OSHA	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
NTP	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
ACGIH	Confirmed animal carcinogen with unknown relevance to humans.
hydroquinone	123-31-9

Further information

Possible risk of irreversible effects.

Further data:

Other dangerous properties can not be excluded.

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Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

Toxicity to fish

LC50 Oncorhynchus mykiss (rainbow trout): 12 mg/l; 96 h (IUCLID)

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia magna (Water flea): 43 - 69 mg/l; 48 h (IUCLID)

Toxicity to algae

IC50 Pseudokirchneriella subcapitata (green algae): 9.8 - 31 mg/l; 96 h (IUCLID)

Persistence and degradability

Biodegradability

63 - 74 %; 28 d

OECD Test Guideline 301D

Readily biodegradable.

Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 2.8

(IUCLID) Bioaccumulation is not expected (log Pow <1).

Mobility in soil

Distribution among environmental compartments

log Koc: 1.50

(External MSDS)

Other adverse effects

Stability in water

6.6 - 128 h

Additional ecological information

Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

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SECTION 14. Transport information

Land transport (DOT)

UN number	UN 3056
Proper shipping name	N-HEPTALDEHYDE
Class	3
Packing group	III
Environmentally hazardous	--

Air transport (IATA)

UN number	UN 3056
Proper shipping name	N-HEPTALDEHYDE
Class	3
Packing group	III
Environmentally hazardous	--
Special precautions for user	no

Sea transport (IMDG)

UN number	UN 3056
Proper shipping name	N-HEPTALDEHYDE
Class	3
Packing group	III
Environmentally hazardous	--
Special precautions for user	yes
EmS	F-E S-D

SECTION 15. Regulatory information

United States of America

OSHA Hazards

Combustible Liquid
Skin sensitizer
Carcinogen
Mutagen
Target organ effects
Corrosive to eyes

This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS, and may deviate from the GHS information on the label and in section 2.

SARA 311/312 Hazards

Fire Hazard
Acute Health Hazard
Chronic Health Hazard

SARA 313

The following components are subject to reporting levels established by SARA Title III, Section 313:

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Ingredients

hydroquinone

123-31-9

SARA 302

The following components are subject to reporting levels established by SARA Title III, Section 302:

Ingredients

hydroquinone

123-31-9

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

Massachusetts Right To Know

Ingredients

hydroquinone

Pennsylvania Right To Know

Ingredients

n-heptanal

hydroquinone

New Jersey Right To Know

Ingredients

n-heptanal

hydroquinone

Notification status

TSCA:

On TSCA Inventory

DSL:

All components of this product are on the Canadian DSL.

SECTION 16. Other information

Training advice

Provide adequate information, instruction and training for operators.

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

H226

Flammable liquid and vapor.

H317

May cause an allergic skin reaction.

H341

Suspected of causing genetic defects.

H351

Suspected of causing cancer.

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

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The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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