

# SAFETY DATA SHEET

Version 6.11  
Revision Date 08/05/2024  
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## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : Heptane  
Product Number : 246654  
Brand : Sigma-Aldrich  
Index-No. : 601-008-00-2  
CAS-No. : 142-82-5

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

Identified uses : Laboratory chemicals, Synthesis of substances  
Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

### 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES  
Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

### 1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

#### GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 2), H225  
Skin irritation (Category 2), H315  
Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336

Sigma-Aldrich - 246654

Page 1 of 11

Aspiration hazard (Category 1), H304  
Short-term (acute) aquatic hazard (Category 1), H400  
Long-term (chronic) aquatic hazard (Category 1), H410

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

Danger

Hazard Statements

H225 Highly flammable liquid and vapor.  
H304 May be fatal if swallowed and enters airways.  
H315 Causes skin irritation.  
H336 May cause drowsiness or dizziness.  
H410 Very toxic to aquatic life with long lasting effects.

Precautionary Statements

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.  
P261 Avoid breathing mist or vapors.  
P264 Wash skin thoroughly after handling.  
P271 Use only outdoors or in a well-ventilated area.  
P273 Avoid release to the environment.  
P280 Wear protective gloves/ eye protection/ face protection.  
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor.  
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.  
P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.  
P331 Do NOT induce vomiting.  
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.  
P391 Collect spillage.  
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.  
P403 + P235 Store in a well-ventilated place. Keep cool.  
P405 Store locked up.  
P501 Dispose of contents/ container to an approved waste disposal plant.

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

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Formula : C<sub>7</sub>H<sub>16</sub>  
Molecular weight : 100.20 g/mol  
CAS-No. : 142-82-5  
EC-No. : 205-563-8  
Index-No. : 601-008-00-2

Component	Classification	Concentration
<b>n-heptane</b>		
	Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 1; H225, H315, H336, H304, H400, H410 Concentration limits: 20 %: STOT SE 3, H336; M-Factor - Aquatic Acute: 1 - Aquatic Chronic: 1	<= 100 %

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

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

No data available

### 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

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

No data available

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides  
Flash back possible over considerable distance.  
Combustible.

### 5.3 Advice for firefighters

No data available

### 5.4 Further information

In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.

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## **SECTION 6: Accidental release measures**

### **6.1 Personal precautions, protective equipment and emergency procedures**

For personal protection see section 8.

### **6.2 Environmental precautions**

No data available

### **6.3 Methods and materials for containment and cleaning up**

No data available

### **6.4 Reference to other sections**

For disposal see section 13.

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## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

For precautions see section 2.2.

### **7.2 Conditions for safe storage, including any incompatibilities**

#### **Storage conditions**

Store under inert gas.

#### **Storage class**

Storage class (TRGS 510): 3: Flammable liquids

### **7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Ingredients with workplace control parameters**

Component	CAS-No.	Value	Control parameters	Basis
n-heptane	142-82-5	TWA	85 ppm 350 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		C	440 ppm 1,800 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		TWA	500 ppm 2,000 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		PEL	400 ppm 1,600 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	500 ppm 2,000 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		TWA	400 ppm	USA. ACGIH Threshold Limit Values (TLV)
		STEL	500 ppm	USA. ACGIH Threshold Limit Values (TLV)

## 8.2 Exposure controls

### Personal protective equipment

#### Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 480 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.2 mm

Break through time: 60 min

Material tested: Dermatril® P (KCL 743 / Aldrich Z677388, Size M)

#### Control of environmental exposure

Prevent product from entering drains.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/ range: -91 °C (-132 °F)
f) Initial boiling point and boiling range	98 °C 208 °F
g) Flash point	-4 °C (25 °F) - closed cup - c.c.
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 7 %(V) Lower explosion limit: 1.1 %(V)
k) Vapor pressure	48 hPa at 20.0 °C (68.0 °F)
l) Vapor density	No data available
m) Density	0.684 g/mL at 25 °C (77 °F)
Relative density	No data available
n) Water solubility	insoluble
o) Partition coefficient: n-octanol/water	log Pow: > 3 - Bioaccumulation is not expected.
p) Autoignition temperature	223.0 °C (433.4 °F)
q) Decomposition temperature	No data available
r) Viscosity	0.64 mm <sup>2</sup> /s at 20 °C (68 °F) -
s) Explosive properties	Not classified as explosive.
t) Oxidizing properties	none

### 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

Sigma-Aldrich - 246654

Page 6 of 11

## 10.2 Chemical stability

No data available

## 10.3 Possibility of hazardous reactions

Risk of ignition or formation of inflammable gases or vapours with:  
Strong oxidizing agents  
phosphorus  
in the presence of:  
Chlorine

## 10.4 Conditions to avoid

No data available

## 10.5 Incompatible materials

rubber, various plastics

## 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - male and female - > 5,000 mg/kg  
(OECD Test Guideline 401)

Remarks: The value is given in analogy to the following substances: isooctane  
LC50 Inhalation - Rat - male and female - 4 h - > 29.29 mg/l - vapor

(OECD Test Guideline 403)

LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg  
(OECD Test Guideline 402)

Remarks: The value is given in analogy to the following substances: isooctane

#### Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 24 h  
(OECD Test Guideline 404)

Remarks: The value is given in analogy to the following substances: isooctane

Remarks: Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation  
(OECD Test Guideline 405)

Remarks: The value is given in analogy to the following substances: isooctane

#### Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative  
(OECD Test Guideline 406)

Remarks: **Germ cell mutagenicity**

Test Type: Ames test  
Test system: Escherichia coli/Salmonella typhimurium  
Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 471  
Result: negative  
Test Type: Chromosome aberration test in vitro  
Test system: rat hepatocytes  
Method: OECD Test Guideline 473  
Result: negative

### **Carcinogenicity**

This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

- 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.
- 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.
- OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

### **Reproductive toxicity**

No data available

### **Specific target organ toxicity - single exposure**

May cause drowsiness or dizziness.

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

### **Specific target organ toxicity - repeated exposure**

No data available

### **Aspiration hazard**

May be fatal if swallowed and enters airways.

Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

## **11.2 Additional Information**

RTECS: MI7700000

Prolonged or repeated exposure to skin causes defatting and dermatitis., Central nervous system depression, narcosis, Damage to the lungs.

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

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

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## **SECTION 12: Ecological information**

### **12.1 Toxicity**

Toxicity to fish                      LL50 - Rainbow darter (*Etheostoma caeruleum*) - > 13.4 mg/l - 96 h  
(OECD Test Guideline 203)

Sigma-Aldrich - 246654

Page 8 of 11



Remarks: (ECHA)

Toxicity to daphnia and other aquatic invertebrates static test EC50 - Daphnia magna (Water flea) - 0.23 mg/l - 21 d  
Remarks: (ECHA)  
(in analogy to similar products)

Toxicity to algae EL50 - Pseudokirchneriella subcapitata (green algae) - 29 mg/l - 72 h  
(OECD Test Guideline 201)  
Remarks: (ECHA)

NOELR - Pseudokirchneriella subcapitata (green algae) - 6.3 mg/l - 72 h  
(OECD Test Guideline 201)  
Remarks: (ECHA)

## 12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 10 d  
Result: 70 % - Readily biodegradable.  
Remarks: (ECHA)

Biochemical Oxygen Demand (BOD) 1,920 mg/g  
Remarks: (IUCLID)

Theoretical oxygen demand 3,500 mg/g  
Remarks: (Lit.)

Ratio BOD/ThBOD 55 %  
Remarks: (Lit.)

## 12.3 Bioaccumulative potential

Indication of bioaccumulation.

## 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 Endocrine disrupting properties

No data available

## 12.7 Other adverse effects

Additional ecological information Do not empty into drains. Avoid release to the environment.

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**SECTION 13: Disposal considerations****13.1 Waste treatment methods**

No data available

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**SECTION 14: Transport information****DOT (US)**

UN number: 1206 Class: 3 Packing group: II  
Proper shipping name: Heptanes  
Reportable Quantity (RQ):  
Marine pollutant: yes Poison Inhalation Hazard: No

**IMDG**

UN number: 1206 Class: 3 Packing group: II EMS-No: F-E, S-D  
Proper shipping name: HEPTANES  
Marine pollutant : yes  
Marine pollutant : yes

**IATA**

UN number: 1206 Class: 3 Packing group: II  
Proper shipping name: Heptanes

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**SECTION 15: Regulatory information****CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

**SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

**SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : Fire Hazard  
Acute Health Hazard  
Chronic Health Hazard

**SARA 313** : 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.

**US State Regulations****Massachusetts Right To Know**

n-heptane 142-82-5

**Pennsylvania Right To Know**

n-heptane 142-82-5

Sigma-Aldrich - 246654

Page 10 of 11

**Maine Chemicals of High Concern**

Product does not contain any listed chemicals

**Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

**Washington Chemicals of High Concern**

Product does not contain any listed chemicals

**The ingredients of this product are reported in the following inventories:**

TSCA : All substances listed as active on the TSCA inventory

**TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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**SECTION 16: Other information**

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

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