

## SAFETY DATA SHEET

Version 6.9  
Revision Date 06/30/2021  
Print Date 10/08/2022**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : Pentane

Product Number : 236705

Brand : Sigma-Aldrich

Index-No. : 601-006-00-1

CAS-No. : 109-66-0

**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 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  
Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336  
Aspiration hazard (Category 1), H304  
Short-term (acute) aquatic hazard (Category 2), H401  
Long-term (chronic) aquatic hazard (Category 2), H411

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

Sigma-Aldrich - 236705

Page 1 of 10

Hazard statement(s)	
H225	Highly flammable liquid and vapor.
H304	May be fatal if swallowed and enters airways.
H336	May cause drowsiness or dizziness.
H411	Toxic 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.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
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.
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

Repeated exposure may cause skin dryness or cracking.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Formula	: C <sub>5</sub> H <sub>12</sub>
Molecular weight	: 72.15 g/mol
CAS-No.	: 109-66-0
EC-No.	: 203-692-4
Index-No.	: 601-006-00-1

Component	Classification	Concentration
<b>pentane</b>	Flam. Liq. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 2; H225, H336, H304, H401, H411 Concentration limits:	<= 100 %

Sigma-Aldrich - 236705

Page 2 of 10

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

---

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. Call in physician.

#### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Remove contact lenses.

#### If swallowed

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

### 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

---

## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Carbon dioxide (CO<sub>2</sub>) Foam Dry powder

#### Unsuitable extinguishing media

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

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

Carbon oxides

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Risk of dust explosion.

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

Forms explosive mixtures with air at ambient temperatures.

### 5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

### 5.4 Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

---

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

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

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

### **6.2 Environmental precautions**

Do not let product enter drains. Risk of explosion.

### **6.3 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 carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

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

For disposal see section 13.

---

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

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

#### **Advice on safe handling**

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

#### **Advice on protection against fire and explosion**

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

#### **Hygiene measures**

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

For precautions see section 2.2.

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

#### **Storage conditions**

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

Refrigerate before opening.

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

---

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

### **8.1 Control parameters**

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

Component	CAS-No.	Value	Control parameters	Basis
pentane	109-66-0	C	610 ppm 1,800 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		TWA	120 ppm 350 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		TWA	1,000 ppm 2,950 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		TWA	600 ppm 1,800 mg/m <sup>3</sup>	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		STEL	750 ppm 2,250 mg/m <sup>3</sup>	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		PEL	600 ppm 1,800 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		TWA	1,000 ppm	USA. ACGIH Threshold Limit Values (TLV)

## 8.2 Exposure controls

### Appropriate engineering controls

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

### Personal protective equipment

#### Eye/face protection

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

#### Skin protection

required

#### Body Protection

Flame retardant antistatic protective clothing.

#### Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

#### Control of environmental exposure

Do not let product enter drains. Risk of explosion.

---

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |                   |   |
|-------------------|---|
| a) Appearance     | Form: clear, liquid<br>Color: colorless |
| b) Odor           | benzine-like                            |
| c) Odor Threshold | No data available                       |

Sigma-Aldrich - 236705

Page 5 of 10

d) pH	No data available
e) Melting point/freezing point	Melting point/range: -130 °C (-202 °F) - lit.
f) Initial boiling point and boiling range	35 - 36 °C 95 - 97 °F - lit.
g) Flash point	-40 °C (-40 °F)
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 8 %(V) Lower explosion limit: 1.4 %(V)
k) Vapor pressure	585.9 hPa at 21.13 °C (70.03 °F)
l) Vapor density	2.49 - (refers to pure substance)
m) Relative density	No data available
n) Water solubility	0.038 g/l at 20 °C (68 °F) - partly soluble
o) Partition coefficient: n-octanol/water	log Pow: 3.45 at 25 °C (77 °F) - Bioaccumulation is not expected.
p) Autoignition temperature	260.0 °C (500.0 °F)
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

Surface tension	ca.15.49 mN/m at 25 °C (77 °F)
Relative vapor density	2.49 - (refers to pure substance)

---

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Vapors may form explosive mixture with air.

### 10.2 Chemical stability

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

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:

Nitric acid

Strong oxidizing agents

halogens

#### 10.4 Conditions to avoid

Warming.

#### 10.5 Incompatible materials

rubber, various plastics

#### 10.6 Hazardous decomposition products

In the event of fire: see section 5

---

### SECTION 11: Toxicological information

#### 11.1 Information on toxicological effects

##### Acute toxicity

LD50 Oral - Rat - male and female - > 2,000 mg/kg  
(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - > 25.3 mg/l  
(OECD Test Guideline 403)

Remarks: (in analogy to similar products)

The value is given in analogy to the following substances: cyclopentane

Dermal: No data available

No data available

##### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

##### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

##### Respiratory or skin sensitization

Buehler Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

##### Germ cell mutagenicity

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: Regulation (EC) No. 440/2008, Annex, B.10

Result: negative

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: In vivo micronucleus test

Species: Rat

Cell type: Bone marrow

Application Route: inhalation (vapor)

Method: Mutagenicity (micronucleus test)

Result: negative

## 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.

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. - Central nervous system

## 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: RZ9450000

Contact with eyes can cause:, Redness, Blurred vision, Provokes tears., Prolonged or repeated contact with skin may cause:, defatting, Dermatitis, Central nervous system depression, 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

---

## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish                      static test LC50 - Oncorhynchus mykiss (rainbow trout) - 4.26 mg/l  
- 96 h  
(OECD Test Guideline 203)

Toxicity to daphnia                      static test EC50 - Daphnia magna (Water flea) - 2.7 mg/l - 48 h  
and other aquatic                      Remarks: (ECHA)  
invertebrates

Toxicity to algae                      static test ErC50 - Selenastrum capricornutum (green algae) - 10.7  
mg/l - 72 h  
(OECD Test Guideline 201)

static test NOEC - Selenastrum capricornutum (green algae) - 7.51  
mg/l - 72 h  
(OECD Test Guideline 201)

### 12.2 Persistence and degradability

Biodegradability                      aerobic - Exposure time 28 d  
Result: 87 % - Readily biodegradable.

Sigma-Aldrich - 236705

Page 8 of 10



### 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

Avoid release to the environment. Do not empty into drains.

---

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

---

## SECTION 14: Transport information

#### DOT (US)

UN number: 1265 Class: 3 Packing group: I  
Proper shipping name: Pentanes  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

#### IMDG

UN number: 1265 Class: 3 Packing group: I EMS-No: F-E, S-D  
Proper shipping name: PENTANES  
Marine pollutant : yes

#### IATA

UN number: 1265 Class: 3 Packing group: I  
Proper shipping name: Pentanes

---

## SECTION 15: Regulatory information

#### SARA 302 Components

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

#### 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, Chronic Health Hazard

## Massachusetts Right To Know Components

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

---

### SECTION 16: Other information

#### Further information

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 Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

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).

Version: 6.9

Revision Date: 06/30/2021

Print Date: 10/08/2022