

# SAFETY DATA SHEET

Version 6.14  
Revision Date 09/08/2024  
Print Date 09/09/2024

## 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  
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  
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

Hazard Statements

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 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.  
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.

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Formula : C<sub>5</sub>H<sub>12</sub>  
Molecular weight : 72.15 g/mol

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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: 20 %: STOT SE 3, H336;	<= 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

#### 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

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## 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.

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## 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.

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.

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## 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.

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## 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

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
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
		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

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: 0.11 mm

Break through time: 10 min

Material tested: KCL 741 Dermatril® L

### Body Protection

Flame retardant antistatic protective clothing.

### Respiratory protection

Recommended Filter type: Filter type AX

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

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.

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## 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                              |
| 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                             | Upper explosion limit: 8 %(V)                  |

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flammability or explosive limits	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) Density	0.626 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.
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	none

## 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)

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## 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

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## 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 - vapor

(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

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## **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 and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 2.7 mg/l - 48 h Remarks: (ECHA)
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.
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**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 Endocrine disrupting properties**

No data available

**12.7 Other adverse effects**

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

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**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.

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**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

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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  
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**

pentane 109-66-0

**Pennsylvania Right To Know**

pentane 109-66-0

**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****Further information**

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its

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