

# SAFETY DATA SHEET

Version 6.8  
Revision Date 08/06/2024  
Print Date 08/07/2024

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : Hexadecane  
Product Number : H6703  
Brand : Sigma-Aldrich  
CAS-No. : 544-76-3

### 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)

Aspiration hazard (Category 1), H304

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

### 2.2 GHS Label elements, including precautionary statements

Sigma-Aldrich - H6703

Page 1 of 10

Pictogram



Signal Word

Danger

Hazard Statements

H304

May be fatal if swallowed and enters airways.

Precautionary Statements

P301 + P310

IF SWALLOWED: Immediately call a POISON CENTER/ doctor.

P331

Do NOT induce vomiting.

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

---

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms : Cetane

Formula : C<sub>16</sub>H<sub>34</sub>  
Molecular weight : 226.44 g/mol  
CAS-No. : 544-76-3  
EC-No. : 208-878-9

Component	Classification	Concentration
<b>n-hexadecane</b>	Asp. Tox. 1; H304	<= 100 %

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

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

---

## **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.

### **5.3 Advice for firefighters**

No data available

### **5.4 Further information**

No data available

---

## **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.

---

## **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**

Hygroscopic. Handle and store under inert gas.

#### **Storage class**

Storage class (TRGS 510): 10: Combustible 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

Contains no substances with occupational exposure limit values.

### 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: 0.11 mm

Break through time: 30 min

Material tested: KCL 741 Dermatril® L

##### Control of environmental exposure

Prevent product from entering drains.

---

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |  |  |
|--|--|
| a) Appearance                              | Form: liquid<br>Color: colorless           |
| b) Odor                                    | odorless                                   |
| c) Odor Threshold                          | Not applicable                             |
| d) pH                                      | No data available                          |
| e) Melting point/freezing point            | Melting point/ range: 18 °C (64 °F) - lit. |
| f) Initial boiling point and boiling range | 287 °C 549 °F - lit.                       |

g) Flash point	112 °C (234 °F) - Regulation (EC) No. 440/2008, Annex, A.9
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	0.004 hPa at 20 °C (68 °F) - Regulation (EC) No. 440/2008, Annex, A.4
l) Vapor density	7.82 - (Air = 1.0)
m) Density	0.773 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	insoluble
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	4.29 mm <sup>2</sup> /s at 20 °C (68 °F) -
s) Explosive properties	No data available
t) Oxidizing properties	none

## 9.2 Other safety information

Surface tension	24.47 mN/m at 25 °C (77 °F) - Surface tension
Relative vapor density	7.82 - (Air = 1.0)

---

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

No data available

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:  
Strong oxidizing agents

### 10.4 Conditions to avoid

No data available

## 10.5 Incompatible materials

Strong oxidizing agents

## 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 - > 5,000 mg/kg

(OECD Test Guideline 401)

Inhalation: No data available

LD50 Dermal - Rabbit - male and female - > 3,160 mg/kg

(OECD Test Guideline 402)

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 - 24 h

(OECD Test Guideline 405)

#### Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

#### Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Micronucleus test

Species: Mouse

Cell type: Red blood cells (erythrocytes)

Application Route: Oral

Method: OECD Test Guideline 474

Result: negative

Remarks: (in analogy to similar products)

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

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

Species: Rat

Cell type: Bone marrow

Application Route: Intraperitoneal

Method: OECD Test Guideline 475  
Result: negative  
Remarks: (in analogy to similar products)

Test Type: dominant lethal test  
Species: Mouse  
Cell type: sperm  
Application Route: Inhalation  
Method: OECD Test Guideline 483  
Result: negative  
Remarks: (in analogy to similar products)

### **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**

No data available

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

No data available

### **Aspiration hazard**

May be fatal if swallowed and enters airways.

## **11.2 Additional Information**

Repeated dose toxicity - Rat - male and female - Oral - 13 Weeks - NOAEL (No observed adverse effect level) -  $\geq$  5,000 mg/kg  
Remarks: (in analogy to similar products)

Repeated dose toxicity - Rat - male and female - Dermal - NOAEL (No observed adverse effect level) -  $>$  495 mg/kg  
Remarks: (in analogy to similar products)

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

After absorption of large quantities:

narcosis

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

---

## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish	semi-static test LL50 - Fish - > 1,028 mg/l - 96 h Remarks: (in analogy to similar products)
Toxicity to daphnia and other aquatic invertebrates	Remarks: (in analogy to similar products) (n-hexadecane)
Toxicity to algae	EL50 - Pseudokirchneriella subcapitata (green algae) - > 3,200 mg/l - 72 h Remarks: (in analogy to similar products) (n-hexadecane)
Toxicity to bacteria	

### 12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 74 % - Readily biodegradable. (OECD Test Guideline 306)
------------------	--

### 12.3 Bioaccumulative potential

Bioaccumulation	Salmo salar (Atlantic salmon) - 7 d - 1700 µg/l(n-hexadecane)  Bioconcentration factor (BCF): 5.6
-----------------	--

### 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

No data available

---

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

No data available



---

## SECTION 14: Transport information

### **DOT (US)**

Not dangerous goods

### **IMDG**

Not dangerous goods

### **IATA**

Not dangerous goods

### **Further information**

Not classified as dangerous in the meaning of transport regulations.

---

## 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** : No SARA Hazards

**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**

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

#### **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.

---

**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).

Version: 6.8

Revision Date: 08/06/2024

Print Date: 08/07/2024