

**SAFETY DATA SHEET**

according to Regulation (EC) No. 1907/2006

Version 6.7

Revision Date 01.03.2023

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

**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

REACH No. : 01-2119936836-25-xxxx

CAS-No. : 544-76-3

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

Identified uses : Laboratory chemicals, Manufacture of substances

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

Company : Merck Life Science S.r.l.  
Via Monte Rosa 93  
I-20149 MILANO

Telephone : +39 02 3341 7340

Fax : +39 02 3801 0737

E-mail address : serviziotecnico@merckgroup.com

**1.4 Emergency telephone**

Emergency Phone # : 800-789-767 (CHEMTREC Italia)  
+39-02-4555-7031 (CHEMTREC chiamate internazionali)  
+39 02-6610-1029 (Centro Antiveleni Niguarda Ca' Granda - Milano)

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****Classification according to Regulation (EC) No 1272/2008**

Aspiration hazard (Category 1), H304

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

**2.2 Label elements****Labelling according Regulation (EC) No 1272/2008**

Pictogram



Signal Word

Danger



Hazard statement(s) H304	May be fatal if swallowed and enters airways.
Precautionary statement(s) P301 + P310 P331 P405 P501	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Do NOT induce vomiting. Store locked up. Dispose of contents/ container to an approved waste disposal plant.
Supplemental Hazard information (EU) EUH066	Repeated exposure may cause skin dryness or cracking.

### 2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

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## 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>		
CAS-No.	544-76-3	Asp. Tox. 1; H304
EC-No.	208-878-9	
		<= 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.

#### 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.

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

Carbon oxides

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

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

#### **5.3 Advice for firefighters**

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

#### **5.4 Further information**

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. 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.

#### **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**

For precautions see section 2.2.

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

##### **Storage conditions**



Tightly closed. Keep locked up or in an area accessible only to qualified or authorized persons.

Hygrosopic. 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

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

### **8.1 Control parameters**

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

### **8.2 Exposure controls**

#### **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 EN374 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 EN374 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

##### **Body Protection**

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.

Recommended Filter type: Filter type ABEK



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.

### **Control of environmental exposure**

Do not let product enter drains.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

- |   |   |
|---|---|
| a) Physical state                               | liquid  |
| b) Color  | colorless   |
| c) Odor   | odorless  |
| d) Melting point/freezing point                 | Melting point/range: 18 °C - lit.   |
| e) Initial boiling point and boiling range      | 287 °C - lit.   |
| f) Flammability (solid, gas)                    | No data available   |
| g) Upper/lower flammability or explosive limits | No data available   |
| h) Flash point                                  | 112 °C - Regulation (EC) No. 440/2008, Annex, A.9   |
| i) Autoignition temperature                     | No data available   |
| j) Decomposition temperature                    | No data available   |
| k) pH   | No data available   |
| l) Viscosity                                    | Viscosity, kinematic: 4,29 mm <sup>2</sup> /s at 20 °C<br>Viscosity, dynamic: No data available |
| m) Water solubility                             | insoluble   |
| n) Partition coefficient: n-octanol/water       | No data available   |
| o) Vapor pressure                               | 0,004 hPa at 20 °C - Regulation (EC) No. 440/2008, Annex, A.4                                   |
| p) Density                                      | 0,773 g/cm <sup>3</sup> at 25 °C - lit.   |
| Relative density                                | No data available   |
| q) Relative vapor density                       | No data available   |
| r) Particle characteristics                     | No data available   |
| s) Explosive properties                         | No data available   |



t) Oxidizing properties none

## 9.2 Other safety information

Surface tension	24,47 mN/m at 25 °C - Surface tension
Relative vapor density	7,82 - (Air = 1.0)

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.  
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

### 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:  
Strong oxidizing agents

### 10.4 Conditions to avoid

Strong heating.

### 10.5 Incompatible materials

Strong oxidizing agents

### 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)  
Inhalation: No data available  
LD50 Dermal - Rabbit - male and female - > 3.160 mg/kg  
(OECD Test Guideline 402)

#### 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**

No data available

#### **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**

### **Endocrine disrupting properties**

#### **Product:**

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.



Repeated dose toxicity - Rat - male and female - Oral - 13 Weeks - NOEL (No observed adverse effect level) -  $\geq$  5.000 mg/kg

Remarks: (in analogy to similar products)

Repeated dose toxicity - Rat - male and female - Dermal - NOEL (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.

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## 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  $\mu$ g/l(n-hexadecane)

Bioconcentration factor (BCF): 5,6

### 12.4 Mobility in soil

No data available

### 12.5 Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.







## 15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

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### SECTION 16: Other information

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

EUH066                      Repeated exposure may cause skin dryness or cracking.  
H304                         May be fatal if swallowed and enters airways.

#### Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative



**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.

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