

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.6

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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 : Methyl hexanoate

Product Number : 21599

Brand : Sigma-Aldrich

REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

CAS-No. : 106-70-7

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

Identified uses : Laboratory chemicals, Manufacture of substances

### 1.3

CHEMIKART

### 1.4 Emergency telephone

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

#### Classification according to Regulation (EC) No 1272/2008

Flammable liquids (Category 3), H226

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                        | Warning                                                                                        |
| Hazard statement(s)<br>H226        | Flammable liquid and vapor.                                                                    |
| Precautionary statement(s)<br>P210 | Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. |
| P233                               | Keep container tightly closed.                                                                 |
| P240                               | Ground and bond container and receiving equipment.                                             |
| P241                               | Use explosion-proof electrical/ ventilating/ lighting/ equipment.                              |
| P242                               | Use non-sparking tools.                                                                        |
| P243                               | Take action to prevent static discharges.                                                      |
| Supplemental Hazard Statements     | none                                                                                           |

### Reduced Labeling (<= 125 ml)

Pictogram

|                                |         |
|--------------------------------|---------|
| Signal Word                    | Warning |
| Hazard statement(s)            | none    |
| Precautionary statement(s)     | none    |
| Supplemental Hazard Statements | none    |

### 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 : Methyl caproate  
Caproic acid methyl ester

Formula : C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>  
Molecular weight : 130,18 g/mol  
CAS-No. : 106-70-7  
EC-No. : 203-425-1

No components need to be disclosed according to the applicable regulations.

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: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

### 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 at elevated temperatures.

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

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. 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 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 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. 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.

#### **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**

### **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: butyl-rubber

Minimum layer thickness: 0,7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

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: Viton®

Minimum layer thickness: 0,7 mm

Break through time: 120 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

### **Body Protection**

Flame retardant antistatic protective clothing.

### **Respiratory protection**

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

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. Risk of explosion.

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

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

- |                                            |                       |
|--------------------------------------------|-----------------------|
| a) Physical state                          | liquid, clear         |
| b) Color                                   | colorless             |
| c) Odor                                    | No data available     |
| d) Melting point/freezing point            | -71,0 °C              |
| e) Initial boiling point and boiling range | 149,5 °C at 1.013 hPa |
| f) Flammability (solid, gas)               | No data available     |

|                                                 |                                                                                   |
|-------------------------------------------------|-----------------------------------------------------------------------------------|
| g) Upper/lower flammability or explosive limits | No data available                                                                 |
| h) Flash point                                  | 37,5 °C - closed cup - 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: No data available<br>Viscosity, dynamic: 1,2 mPa.s at 20 °C |
| m) Water solubility                             | 1,33 g/l at 20 °C                                                                 |
| n) Partition coefficient: n-octanol/water       | log Pow: 2,34 at 25 °C - Bioaccumulation is not expected.                         |
| o) Vapor pressure                               | 5 hPa at 25 °C                                                                    |
| p) Density                                      | 0,884 g/mL at 20 °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

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

### 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

Strong acids

strong alkalis

### 10.4 Conditions to avoid

Heating.

## 10.5 Incompatible materials

No data available

## 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 - > 5 mg/l - aerosol

(OECD Test Guideline 436)

Dermal: 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

Buehler Test - Guinea pig

Result: Does not cause skin sensitization.

(OECD Test Guideline 406)

#### Germ cell mutagenicity

No data available

#### 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

No data available

### 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.

RTECS: MO8401400

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

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## SECTION 12: Ecological information

### 12.1 Toxicity

|                                                                       |                                                                                                                                 |
|-----------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------|
| Toxicity to daphnia and other aquatic invertebrates                   | semi-static test EC50 - Daphnia magna (Water flea) - 40 mg/l - 48 h (OECD Test Guideline 202)                                   |
|                                                                       | semi-static test NOEC - Daphnia magna (Water flea) - 25 mg/l - 48 h (OECD Test Guideline 202)                                   |
| Toxicity to algae                                                     | static test ErC50 - Pseudokirchneriella subcapitata - 61 mg/l - 72 h (OECD Test Guideline 201)                                  |
|                                                                       | static test NOEC - Pseudokirchneriella subcapitata - 12,5 mg/l - 72 h (OECD Test Guideline 201)                                 |
| Toxicity to bacteria                                                  | static test EC50 - activated sludge - > 1.000 mg/l - 3 h (OECD Test Guideline 209)<br>Remarks: (in analogy to similar products) |
| Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity) | semi-static test NOEC - Daphnia magna (Water flea) - 1,8 mg/l - 21 d (OECD Test Guideline 211)                                  |

### 12.2 Persistence and degradability

|                  |                                                                                                                                                  |
|------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|
| Biodegradability | aerobic - Exposure time 28 d<br>Result: 78 % - Readily biodegradable.<br>(OECD Test Guideline 301C)<br>Remarks: (in analogy to similar products) |
|------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|

### 12.3 Bioaccumulative potential

No data available

### 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.

## 12.6 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.

## 12.7 Other adverse effects

No data available

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

No data available

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## SECTION 14: Transport information

### 14.1 UN number

ADR/RID: 3272

IMDG: 3272

IATA: 3272

### 14.2 UN proper shipping name

ADR/RID: ESTERS, N.O.S. (methyl hexanoate)

IMDG: ESTERS, N.O.S. (methyl hexanoate)

IATA: Esters, n.o.s. (methyl hexanoate)

### 14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA: 3

### 14.4 Packaging group

ADR/RID: III

IMDG: III

IATA: III

### 14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

### 14.6 Special precautions for user

Tunnel restriction code : (D/E)

Further information : No data available

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## SECTION 15: Regulatory information

### 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

#### **National legislation**

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council P5c FLAMMABLE LIQUIDS

on the control of major-accident hazards involving dangerous substances.

### **Other regulations**

Take note of Dir 94/33/EC on the protection of young people at work.

## **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.**

H226                      Flammable liquid and vapor.

### **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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