

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.7

Revision Date 07.06.2023

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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 : 4-Hydroxy-4-methyl-2-pentanone

Product Number : 78891

Brand : Sigma-Aldrich

Index-No. : 603-016-00-1

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. : 123-42-2

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

Eye irritation (Category 2), H319

Reproductive toxicity (Category 2), H361fd

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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) | |
| H226 | Flammable liquid and vapor. |
| H319 | Causes serious eye irritation. |
| H335 | May cause respiratory irritation. |
| H361fd | Suspected of damaging fertility. Suspected of damaging the unborn child. |
| Precautionary statement(s) | |
| P202 | Do not handle until all safety precautions have been read and understood. |
| 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. |
| P305 + P351 + P338 | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. |
| P308 + P313 | IF exposed or concerned: Get medical advice/ attention. |
| Supplemental Hazard Statements | none |

Reduced Labeling (<= 125 ml)

Pictogram

| | |
|--------------------------------|---|
| Signal Word | Warning |
| Hazard statement(s) | |
| H361fd | Suspected of damaging fertility. Suspected of damaging the unborn child. |
| Precautionary statement(s) | |
| P202 | Do not handle until all safety precautions have been read and understood. |
| P308 + P313 | IF exposed or concerned: Get medical advice/ attention. |
| 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.

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula : C₆H₁₂O₂
Molecular weight : 116,16 g/mol
CAS-No. : 123-42-2
EC-No. : 204-626-7
Index-No. : 603-016-00-1

| Component | | Classification | Concentration |
|----------------------------------|--------------|--|---------------|
| 2-Methyl-2-pentanol-4-one | | | |
| CAS-No. | 123-42-2 | Flam. Liq. 3; Eye Irrit. 2; Repr. 2; STOT SE 3; H226, H319, H361fd, H335 Concentration limits: >= 10 %: Eye Irrit. 2, H319; | <= 100 % |
| EC-No. | 204-626-7 | | |
| Index-No. | 603-016-00-1 | | |

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. Consult a physician.

In case of eye contact

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

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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

Foam Carbon dioxide (CO₂) 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

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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 with liquid-absorbent material (e.g. Chemisorb®).

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 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.

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

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).

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).

Splash contact

Material: Chloroprene

Minimum layer thickness: 0,65 mm

Break through time: 240 min

Material tested: KCL 720 Camapren®

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.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---|--|
| a) Physical state | clear, liquid |
| b) Color | light yellow, colorless |
| c) Odor | No data available |
| d) Melting point/freezing point | Melting point: -44 °C |
| e) Initial boiling point and boiling range | 158 - 162 °C at 1.013,25 hPa |
| f) Flammability (solid, gas) | No data available |
| g) Upper/lower flammability or explosive limits | Upper explosion limit: 6,9 %(V) Lower explosion limit: 1,8 %(V) |
| h) Flash point | 58 °C - closed cup |
| i) Autoignition temperature | No data available |
| j) Decomposition temperature | No data available |
| k) pH | No data available |
| l) Viscosity | Viscosity, kinematic: No data available Viscosity, dynamic: No data available |
| m) Water solubility | No data available |
| n) Partition coefficient: n-octanol/water | No data available |
| o) Vapor pressure | No data available |
| p) Density | 0,938 g/cm ³ at 20 °C |
| 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

Relative vapor density 4,01 - (Air = 1.0)

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

No data available

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

various plastics, 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 - 3.002 mg/kg
(OECD Test Guideline 401)

Symptoms: Risk of aspiration upon vomiting., Aspiration may cause pulmonary edema and pneumonitis.

Symptoms: mucosal irritations

LD50 Dermal - Rabbit - 13.630 mg/kg

Remarks: (IUCLID)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 24 h

(OECD Test Guideline 404)

Remarks: (IUCLID)

Remarks: Drying-out effect resulting in rough and chapped skin.

Remarks: Dermatitis

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irritating to eyes.

(OECD Test Guideline 405)

Remarks: (IUCLID)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster lung cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

Suspected of damaging the unborn child.

Suspected of damaging fertility.

Specific target organ toxicity - single exposure

May cause respiratory irritation. - Respiratory Tract

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.

Repeated dose toxicity - Rat - male and female - Oral - 13 Weeks - NOAEL (No observed adverse effect level) - 600 mg/kg

RTECS: SA9100000

Central nervous system depression, Symptoms and signs include headache, dizziness, fatigue, muscular weakness, drowsiness and in extreme cases, loss of consciousness., Blood disorders, Dermatitis, Blurred vision, Effects due to ingestion may include: To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption of large quantities:

narcosis
respiratory arrest
Convulsions

Possible damages:

Damage to:

Liver
Kidney
Central nervous system

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity

| | |
|---|--|
| Toxicity to fish | semi-static test LC50 - <i>Oryzias latipes</i> (Orange-red killifish) - > 100 mg/l - 96 h (OECD Test Guideline 203) |
| Toxicity to daphnia and other aquatic invertebrates | semi-static test EC50 - <i>Daphnia magna</i> (Water flea) - > 1.000 mg/l - 48 h (OECD Test Guideline 202) semi-static test NOEC - <i>Daphnia magna</i> (Water flea) - > 1.000 mg/l - 48 h (OECD Test Guideline 202) |
| Toxicity to algae | static test ErC50 - <i>Pseudokirchneriella subcapitata</i> (green algae) - > 1.000 mg/l - 72 h (OECD Test Guideline 201) static test NOEC - <i>Pseudokirchneriella subcapitata</i> (green algae) - >= 1.000 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) |
| Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity) | semi-static test LC50 - <i>Daphnia magna</i> (Water flea) - > 100 mg/l - 21 d (OECD Test Guideline 211) |

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
Result: 98,51 % - Readily biodegradable.
(OECD Test Guideline 301A)

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

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1148 IMDG: 1148 IATA: 1148

14.2 UN proper shipping name

ADR/RID: DIACETONE ALCOHOL
IMDG: DIACETONE ALCOHOL
IATA: Diacetone alcohol

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

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.

Authorisations and/or restrictions on use

National legislation

Seveso III: Directive 2012/18/EU of the P5c FLAMMABLE LIQUIDS
European Parliament and of the Council
on the control of major-accident hazards
involving dangerous substances.

Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

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

SECTION 16: Other information

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

| | |
|--------|--|
| H226 | Flammable liquid and vapor. |
| H319 | Causes serious eye irritation. |
| H335 | May cause respiratory irritation. |
| H361fd | Suspected of damaging fertility. Suspected of damaging the unborn child. |

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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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