



MATERIAL SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Date of issue: 02/05/2013

Version 1.0

SECTION 1. Identification

Product identifier

Product number	804512
Product name	4-Hydroxy-4-methyl-2-pentanone for synthesis

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

Identified uses	Chemical for synthesis
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Details of the supplier of the safety data sheet

Company	EMD Millipore Corporation 290 Concord Road, Billerica, MA 01821, United States of America SDS Phone Support: +1-978-715-1335 General Inquiries: +1-978-715-4321 Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5) e-mail: mm_sds@merckgroup.com
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Emergency telephone	800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week
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SECTION 2. Hazards identification

GHS Classification

Flammable liquid, Category 3, H226

Eye irritation, Category 2, H319

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

GHS-Labeling

Hazard pictograms



Signal Word

Warning

Hazard Statements

H226 Flammable liquid and vapor.

H319 Causes serious eye irritation.

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Precautionary Statements

P210 Keep away from heat.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

OSHA Hazards

This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).

Other hazards

None known.

SECTION 3. Composition/information on ingredients

Formula	$(\text{CH}_3)_2\text{C}(\text{OH})\text{CH}_2\text{COCH}_3$	$\text{C}_6\text{H}_{12}\text{O}_2$ (Hill)
CAS-No.	123-42-2	
Molar mass	116.16 g/mol	

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.

4-hydroxy-4-methylpentan-2-one ($\geq 90\%$ - $\leq 100\%$)

123-42-2

SECTION 4. First aid measures

Description of first-aid measures

Inhalation

After inhalation: fresh air.

Skin contact

After skin contact: wash off with plenty of water. Remove contaminated clothing.

Eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist.

Ingestion

If swallowed Caution Aspiration hazard Keep respiratory tract clear. Call a physician immediately.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

irritant effects, respiratory arrest, Dermatitis, narcosis, Convulsions

Drying-out effect resulting in rough and chapped skin.

Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂), Foam, Dry powder

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Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

Special hazards arising from the substance or mixture

Combustible material

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

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

Advice for firefighters

Special protective equipment for fire-fighters

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

Further information

Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

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.

Advice for emergency responders: Protective equipment see section 8.

Environmental precautions

Do not empty into drains. Risk of explosion.

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.

SECTION 7. Handling and storage

Precautions for safe handling

Observe label precautions.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Store at +15°C to +25°C (+59°F to +77°F).

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SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Ingredients

Basis	Value	Threshold limits	Remarks
<i>4-hydroxy-4-methylpentan-2-one 123-42-2</i>			
ACGIH	Time Weighted Average (TWA):	50 ppm	
NIOSH/GUIDE	Recommended exposure limit (REL):	50 ppm 240 mg/m ³	
OSHA_TRANS	PEL:	50 ppm 240 mg/m ³	
Z1A	Time Weighted Average (TWA):	50 ppm 240 mg/m ³	

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures

Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance.

Eye/face protection

Safety glasses

Hand protection

Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Other protective equipment:

Flame retardant antistatic protective clothing

Respiratory protection

required when vapors/aerosols are generated.

Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

SECTION 9. Physical and chemical properties

Physical state	liquid
Color	colorless
Odor	pleasant

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Odor Threshold	0.3 - 99.4 ppm
pH	No information available.
Melting point	-47 °C
Boiling point/boiling range	334 °F (168 °C)
Flash point	136 °F (58 °C) Method: DIN 51755 Part 1
Evaporation rate	No information available.
Flammability (solid, gas)	not applicable
Lower explosion limit	1.8 %(V)
Upper explosion limit	6.9 %(V)
Vapor pressure	1.1 hPa at 68 °F (20 °C)
Relative vapor density	4.0
Relative density	0.94 g/cm ³ at 68 °F (20 °C)
Water solubility	at 68 °F (20 °C) soluble
Partition coefficient: n-octanol/water	log Pow: 1.03 (calculated) (IUCLID) Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.
Decomposition temperature	> 194 °F (> 90 °C)
Viscosity, dynamic	3.22 mPa.s at 68 °F (20 °C)
Explosive properties	Not classified as explosive.
Ignition temperature	1184 °F (640 °C)

SECTION 10. Stability and reactivity

Reactivity

Vapor/air-mixtures are explosive at intense warming.

Chemical stability

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The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions

Violent reactions possible with:

Risk of ignition or formation of inflammable gases or vapors with:

Oxidizing agents, Alcohols, Amines, Alkali metals, acids

Conditions to avoid

Heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

Incompatible materials

various plastics

Hazardous decomposition products

no information available

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure

Inhalation, Eye contact, Skin contact

Target Organs

Eyes

Skin

Respiratory system

Central nervous system

Liver

Acute oral toxicity

LD50 rat: 2,520 mg/kg (RTECS)

Symptoms: Convulsions

Acute inhalation toxicity

Symptoms: mucosal irritations

Acute dermal toxicity

LD50 rabbit: 13,630 mg/kg

(IUCLID)

Skin irritation

rabbit

Result: slight irritation

(IUCLID)

Drying-out effect resulting in rough and chapped skin.

Dermatitis

Eye irritation

rabbit

Result: Severe irritations

(IUCLID)

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Product name

4-Hydroxy-4-methyl-2-pentanone for synthesis

Causes serious eye irritation.

Genotoxicity in vitro

Ames test

Result: negative

(IUCLID)

Specific target organ systemic toxicity - single exposure

The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ systemic toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

Regarding the available data the classification criteria are not fulfilled.

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.

OSHA

No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

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.

ACGIH

No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

Further information

After absorption of large quantities:

narcosis, respiratory arrest

Possible damages:

Damage to:

Liver, Kidney, Central nervous system

Further data:

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

Toxicity to fish

LC50 *Lepomis macrochirus* (Bluegill sunfish): 420 mg/l; 96 h (IUCLID)

Toxicity to daphnia and other aquatic invertebrates

EC50 *Daphnia*: 9,000 mg/l; 24 h (IUCLID)

Toxicity to bacteria

EC *Pseudomonas putida*: 825 mg/l; 16 h (IUCLID)

Persistence and degradability

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Biodegradability

100 %; 14 d

(IUCLID)

Readily biodegradable.

Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 1.03

(calculated)

(IUCLID) Bioaccumulation is not expected (log Pow <1).

Mobility in soil

No information available.

Other adverse effects

Additional ecological information

Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

SECTION 14. Transport information

Land transport (DOT)

UN number

UN 1148

Proper shipping name

DIACETONE ALCOHOL

Class

3

Packing group

III

Environmentally hazardous

--

Air transport (IATA)

UN number

UN 1148

Proper shipping name

DIACETONE ALCOHOL

Class

3

Packing group

III

Environmentally hazardous

--

Special precautions for user

no

Sea transport (IMDG)

UN number

UN 1148

Proper shipping name

DIACETONE ALCOHOL

Class

3

Packing group

III

Environmentally hazardous

--

Special precautions for user

yes

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EmS

F-E S-D

SECTION 15. Regulatory information

United States of America

OSHA Hazards

Combustible Liquid

Eye irritant

Target organ effects

This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS, and may deviate from the GHS information on the label and in section 2.

SARA 311/312 Hazards

Fire Hazard

Acute Health Hazard

Chronic Health Hazard

SARA 313

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.

SARA 302

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

TSCA 12b

Ingredients

4-hydroxy-4-methylpentan-2-one

123-42-2

Massachusetts Right To Know

Ingredients

4-hydroxy-4-methylpentan-2-one

Pennsylvania Right To Know

Ingredients

4-hydroxy-4-methylpentan-2-one

New Jersey Right To Know

Ingredients

4-hydroxy-4-methylpentan-2-one

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Notification status

TSCA: On TSCA Inventory

DSL: All components of this product are on the Canadian DSL.

SECTION 16. Other information

Training advice

Provide adequate information, instruction and training for operators.

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

H226 Flammable liquid and vapor.
H319 Causes serious eye irritation.

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Date of issue:02/05/2013

The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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