



# MATERIAL SAFETY DATA SHEET

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

Date of issue: 03/11/2013

Version 1.0

## SECTION 1. Identification

### Product identifier

Product number	820926
Product name	2-Octanone 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  
Acute toxicity, Category 4, Dermal, H312  
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.  
H312 Harmful in contact with skin.

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## *Precautionary Statements*

P210 Keep away from heat.

P260 Do not breathe vapors.

## **OSHA Hazards**

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

## **Other hazards**

None known.

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## **SECTION 3. Composition/information on ingredients**

Formula	$\text{CH}_3(\text{CH}_2)_5\text{COCH}_3$	$\text{C}_8\text{H}_{16}\text{O}$ (Hill)
CAS-No.	111-13-7	
Molar mass	128.21 g/mol	

## **Hazardous ingredients**

*Chemical Name ( Concentration)*

CAS-No.

*Octan-2-one ( >= 90 % - <= 100 % )*

111-13-7

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## **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. Get medical attention.

#### *Eye contact*

After eye contact: rinse out with plenty of water.

#### *Ingestion*

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

Never give anything by mouth to an unconscious person.

### **Most important symptoms and effects, both acute and delayed**

The following applies to ketones in general: when vapors/aerosols occur, mucosal irritations, coughing, and dyspnoea after inhalation. The absorption of large quantities leads to: CNS depression (narcosis). Repeated skin contact leads to a degreasing effect, with secondary inflammation possible. Toxic effects on the liver and kidneys cannot be excluded after high doses. The inhalation of droplets may result in the formation of oedemas in the respiratory tract.

### **Indication of any immediate medical attention and special treatment needed**

No information available.

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## **SECTION 5. Fire-fighting measures**

### **Extinguishing media**

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### *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.

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

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 vapors possible in the event of fire.

### **Advice for firefighters**

#### *Special protective equipment for fire-fighters*

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

#### *Further information*

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

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## **SECTION 6. Accidental release measures**

### **Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Avoid substance contact. 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.

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.

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## **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)

Contains no substances with occupational exposure limit values.

### 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.

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## SECTION 9. Physical and chemical properties

Physical state	liquid
Color	colorless
Odor	fruity
Odor Threshold	No information available.
pH	No information available.
Melting point	-16 °C
Boiling point/boiling range	342 - 343 °F ( 172 - 173 °C) at 1,013 hPa
Flash point	133 °F ( 56 °C)
Evaporation rate	No information available.

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Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapor pressure	1.8 hPa at 77 °F ( 25 °C)
Relative vapor density	No information available.
Relative density	0.82 g/cm <sup>3</sup> at 68 °F ( 20 °C)
Water solubility	0.9 g/l at 68 °F ( 20 °C)
Partition coefficient: n-octanol/water	log Pow: 2.37 (experimental) (Lit.) Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Ignition temperature	563 °F ( 295 °C)

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### SECTION 10. Stability and reactivity

#### Reactivity

Vapor/air-mixtures are explosive at intense warming.

#### Chemical stability

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

#### Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents, strong reducing agents, Strong bases

#### Conditions to avoid

Heating.

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

#### Incompatible materials

no information available

#### Hazardous decomposition products

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no information available

## SECTION 11. Toxicological information

### Information on toxicological effects

#### *Likely route of exposure*

Inhalation, Eye contact, Skin contact

#### *Acute oral toxicity*

LD50 rat: 3,089 mg/kg (RTECS)

#### *Acute inhalation toxicity*

LC50 rat: 11.400 mg/m<sup>3</sup>; 6 h (RTECS)

#### *Acute dermal toxicity*

LD50 rabbit: 1,337 mg/kg  
(RTECS)

absorption

#### *Genotoxicity in vitro*

Ames test

Result: negative  
(HSDB)

#### *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:

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We have no description of any toxic symptoms.

The following applies to ketones in general: when vapors/aerosols occur, mucosal irritations, coughing, and dyspnoea after inhalation. The absorption of large quantities leads to: CNS depression (narcosis). Repeated skin contact leads to a degreasing effect, with secondary inflammation possible. Toxic effects on the liver and kidneys cannot be excluded after high doses. The inhalation of droplets may result in the formation of oedemas in the respiratory tract.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

## SECTION 12. Ecological information

### Ecotoxicity

*Toxicity to fish*

LC50 Pimephales promelas (fathead minnow): 36 mg/l; 96 h (ECOTOX Database)

### Persistence and degradability

No information available.

### Bioaccumulative potential

*Partition coefficient: n-octanol/water*

log Pow: 2.37

(experimental)

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

### Mobility in soil

No information available.

### Other adverse effects

## 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 1993
Proper shipping name	FLAMMABLE LIQUID, N.O.S. ( 2-OCTANONE)
Class	3
Packing group	III
Environmentally hazardous	--

### Air transport (IATA)

UN number	UN 1993
Proper shipping name	FLAMMABLE LIQUID, N.O.S. ( 2-OCTANONE)
Class	3
Packing group	III
Environmentally hazardous	--

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Special precautions for user	no
Sea transport (IMDG)	
UN number	UN 1993
Proper shipping name	FLAMMABLE LIQUID, N.O.S. ( 2-OCTANONE)
Class	3
Packing group	III
Environmentally hazardous	--
Special precautions for user	yes
EmS	F-E S-E

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### SECTION 15. Regulatory information

#### United States of America

##### OSHA Hazards

Combustible Liquid  
Highly toxic by inhalation  
Harmful by skin absorption.

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

##### 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.

##### DEA List I

Not listed

##### DEA List II

Not listed

##### Massachusetts Right To Know

Remarks

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

##### Pennsylvania Right To Know

*Ingredients*

Octan-2-one



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### New Jersey Right To Know

#### *Ingredients*

Octan-2-one

### Notification status

TSCA: On TSCA Inventory

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

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## 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.  
H312 Harmful in contact with skin.

### 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](http://www.wikipedia.org).

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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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