



MATERIAL SAFETY DATA SHEET

according to the Hazard Communication Standard (29 CFR 1910.1200)

Date of issue: 10/21/2012

Version 1.0

SECTION 1. Identification

Product identifier

Product number 821627
Product name Isooctane for synthesis

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

Identified uses Chemical for synthesis

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

Emergency telephone 800-424-9300 CHEMTREC (USA)
+1-703-527-3887 CHEMTREC (International)
24 Hours/day; 7 Days/week

SECTION 2. Hazards identification

GHS Classification

Flammable liquid, Category 2, H225
Aspiration hazard, Category 1, H304
Skin irritation, Category 2, H315
Specific target organ systemic toxicity - single exposure, Category 3, H336
Acute aquatic toxicity, Category 1, H400
Chronic aquatic toxicity, Category 1, H410

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

GHS-Labeling

Hazard pictograms



Signal Word
Danger

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Hazard Statements

H225 Highly flammable liquid and vapor.
H304 May be fatal if swallowed and enters airways.
H315 Causes skin irritation.
H336 May cause drowsiness or dizziness.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary Statements

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P233 Keep container tightly closed.
P240 Ground/bond container and receiving equipment.
P273 Avoid release to the environment.
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P331 Do NOT induce vomiting.
P403 + P235 Store in a well-ventilated place. Keep cool.

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	$\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_3$	C_8H_{18} (Hill)
CAS-No.	540-84-1	
Molar mass	114.23 g/mol	

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.

isooctane (>= 90 % - <= 100 %)

540-84-1

SECTION 4. First aid measures

Description of first-aid measures

Inhalation

After inhalation: fresh air. Call in physician.

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 with the eyelid held wide open. Call in ophthalmologist if necessary.

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Ingestion

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

irritant effects, Drowsiness, drowsiness

It generally applies for aliphatic hydrocarbons with 6 - 18 carbon atoms that they may cause pneumonia, in some cases also pulmonary oedema, upon direct inhalation, i.e. in conditions that can occur only in very special circumstances (nebulizations, spraying, inhalation of aerosols and similar). After absorption of very large quantities: narcosis.

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

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.

Pay attention to flashback.

Forms explosive mixtures with air at ambient 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

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

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).

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Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. Handling and storage

Precautions for safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapors/aerosols.

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

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

SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Ingredients

Basis	Value	Threshold limits	Remarks
<i>isooctane 540-84-1</i>			
ACGIH	Time Weighted Average (TWA):	300 ppm	
NIOSH/GUIDE	Recommended exposure limit (REL):	75 ppm	
		350 mg/m ³	
OSHA_TRANS	Ceiling Limit Value and Time Period (if specified):	385 ppm	Ceiling Limit Value 15-min
		1,800 mg/m ³	
Z1A	PEL:	500 ppm	
		2,350 mg/m ³	
Z1A	Time Weighted Average (TWA):	300 ppm	
		1,450 mg/m ³	
Z1A	Short Term Exposure Limit (STEL):	375 ppm	
		1,800 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. Work under hood. Do not inhale substance/mixture.

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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.

Recommended:

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0.40 mm
Break through time:	> 480 min

splash contact:

Glove material:	polychloroprene
Glove thickness:	0.65 mm
Break through time:	> 120 min

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	benzine-like
Odor Threshold	No information available.
pH	neutral
Melting point	-161 °F (-107 °C)
Boiling point/boiling range	210 °F (99 °C) at 1,013 hPa
Flash point	10 °F (-12 °C) Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1 %(V)

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Upper explosion limit	6 %(V)
Vapor pressure	51 hPa at 68 °F (20 °C)
Relative vapor density	3.9
Relative density	0.69 g/cm ³ at 68 °F (20 °C)
Water solubility	0.56 mg/l at 77 °F (25 °C)
Partition coefficient: n-octanol/water	log Pow: 4.09 (calculated) Potential bioaccumulation
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	0.50 mPa.s at 68 °F (20 °C)
Ignition temperature	770 °F (410 °C)
Saturated vapor concentration	239 g/m ³ at 68 °F (20 °C)

SECTION 10. Stability and reactivity

Reactivity

Vapors may form explosive mixture with air.

Chemical stability

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

Possibility of hazardous reactions

Violent reactions possible with:
Strong oxidizing agents

Conditions to avoid

Warming.
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

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SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure

Inhalation, Eye contact, Skin contact

Acute oral toxicity

LD50 rat: > 2,500 mg/kg (IUCLID)

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

absorption

Acute inhalation toxicity

LC50 rat: 37.5 mg/l; 4 h (IUCLID)

Symptoms: mucosal irritations

Skin irritation

Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

Causes skin irritation.

Eye irritation

slight irritation

Genotoxicity in vitro

Mutagenicity (mammal cell test):

Result: negative

(IUCLID)

Specific target organ systemic toxicity - single exposure

May cause drowsiness or dizziness.

Specific target organ systemic toxicity - repeated exposure

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

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

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

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carcinogen by ACGIH.

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It generally applies for aliphatic hydrocarbons with 6 - 18 carbon atoms that they may cause pneumonia, in some cases also pulmonary oedema, upon direct inhalation, i.e. in conditions that can occur only in very special circumstances (nebulizations, spraying, inhalation of aerosols and similar). After absorption of very large quantities: narcosis.

Further data:

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

Toxicity to fish

LC0 Leuciscus idus (Golden orfe): 500 mg/l; 48 h (External MSDS)

Toxicity to bacteria

EC0 Pseudomonas putida: 10,000 mg/l (IUCLID)

Persistence and degradability

No information available.

Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 4.09

(calculated)

Potential bioaccumulation

Mobility in soil

Distribution among environmental compartments

log Koc: 4.35

(HSDB) High mobility of the substance in soil is not expected (log koc ≥ 3).

Other adverse effects

Henry constant

305000 Pa \cdot m³/mol

(HSDB) Distribution preferentially in air.

Additional ecological information

Biological effects:

Endangers drinking-water supplies if allowed to enter soil and/or waters in large quantities.

Further information on ecology

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.

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SECTION 14. Transport information

Land transport (DOT)

UN number UN 1262
Proper shipping name OCTANES
Class 3
Packing group II
Environmentally hazardous --

Air transport (IATA)

UN number UN 1262
Proper shipping name OCTANES
Class 3
Packing group II
Environmentally hazardous --
Special precautions for user no

Sea transport (IMDG)

UN number UN 1262
Proper shipping name OCTANES
Class 3
Packing group II
Environmentally hazardous --
Special precautions for user yes
EmS F-E S-E

SECTION 15. Regulatory information

United States of America
OSHA Hazards

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Flammable Liquid
Skin irritant

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.

TSCA list

Not relevant

SARA 311/312 Hazards

Fire Hazard
Acute Health Hazard

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.

Massachusetts Right To Know

Ingredients
isooctane

Pennsylvania Right To Know

Ingredients
isooctane

New Jersey Right To Know

Ingredients
isooctane

California Prop 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

Notification status

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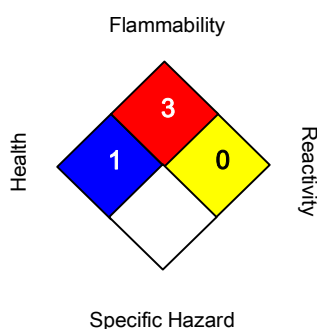
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TSCA: On TSCA Inventory
DSL: All components of this product are on the Canadian DSL.

SECTION 16. Other information

National Fire Protection Association (U.S.A)



Training advice

Provide adequate information, instruction and training for operators.

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

H225	Highly flammable liquid and vapor.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H336	May cause drowsiness or dizziness.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.

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.

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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