



MATERIAL SAFETY DATA SHEET

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

Revision Date 08/21/2013

Version 1.1

SECTION 1. Identification

Product identifier

Product number 803456
Product name 1,4-Diazabicyclo[2.2.2]octane 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)

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 solid, Category 1, H228
Acute toxicity, Category 4, Oral, H302
Skin irritation, Category 2, H315
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
Danger

Hazard Statements

H228 Flammable solid
H302 Harmful if swallowed.
H315 Causes skin irritation.
H319 Causes serious eye irritation.

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Precautionary Statements

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

P260 Do not breathe dust.

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

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	C ₈ H ₁₂ N ₂ (Hill)
CAS-No.	280-57-9
Molar mass	112.17 g/mol

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.

1,4-Diazabicyclo[2.2.2]octane (>= 90 % - <= 100 %)
280-57-9

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

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

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

irritant effects, conjunctivitis, Cough, Shortness of breath, Nausea, Headache, Vertigo

Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Fire-fighting measures

Extinguishing media

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Suitable extinguishing media

Water, 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.

Forms explosive mixtures with air at elevated temperatures.

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

Fire may cause evolution of:

Ammonia, nitrogen oxides

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

Suppress (knock down) gases/vapors/mists with a water spray jet. 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: Avoid substance contact. Avoid inhalation of dusts.

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.

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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

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

Tightly closed. Dry. 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:

protective clothing

Respiratory protection

required when dusts 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	solid
Color	white
Odor	ammoniacal
Odor Threshold	No information available.
pH	at 68 °F (20 °C) alkaline, Aqueous solution
Melting point	155 - 158 °C
Boiling point	No information available.
Flash point	144.0 °F (62.2 °C)
Evaporation rate	No information available.

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Flammability (solid, gas)	Flammable solid
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapor pressure	0.68 hPa at 70 °F (21 °C)
Relative vapor density	No information available.
Relative density	1.14 g/cm ³ at 77 °F (25 °C)
Water solubility	ca. 400 g/l at 68 °F (20 °C)
Partition coefficient: n-octanol/water	log Pow: -0.49 (calculated) (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	No information available.
Ignition temperature	662 °F (350 °C)
Bulk density	800 kg/m ³

SECTION 10. Stability and reactivity

Reactivity

has a corrosive effect
exothermic dissolution process with water
The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

Chemical stability

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

Possibility of hazardous reactions

Caution! In contact with nitrites, nitrates, nitrous acid possible liberation of nitosamines!

Violent reactions possible with:

mineral acids, Strong oxidizing agents, peroxi compounds, iron/iron-containing compounds, acids

Risk of explosion with:

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hydrogen peroxide

Conditions to avoid

Heating.

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

Exposure to moisture.

Incompatible materials

Aluminum, Iron, Copper, Zinc

Hazardous decomposition products

in the event of fire: See section 5.

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure

Inhalation, Eye contact, Skin contact, Ingestion

Acute oral toxicity

LD50 rat: 700 mg/kg (External MSDS)

Symptoms: Nausea

absorption

Acute inhalation toxicity

Symptoms: Possible damages:, mucosal irritations

Skin irritation

rabbit

Result: Irritations

(External MSDS)

Causes skin irritation.

Eye irritation

rabbit

Result: Severe irritations

(External MSDS) Lacrimal irritation due to vapors. conjunctivitis

Causes serious eye irritation.

Genotoxicity in vitro

Mutagenicity (mammal cell test): micronucleus.

Result: negative

(External MSDS)

Ames test

Result: negative

(Lit.)

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.

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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:

Dizziness, Headache

Damage to:

Kidney

Other information

Under given conditions, contact with nitrites or nitric acid can lead to the formation of nitrosamines, which have shown themselves to be carcinogenic in animal experiments.

Further data:

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): 1,730 mg/l; 96 h (ECOTOX Database)

Toxicity to daphnia and other aquatic invertebrates

EC0 Daphnia magna (Water flea): 92 mg/l; 48 h

OECD Test Guideline 202

Toxicity to algae

IC50 Pseudokirchneriella subcapitata (green algae): 180 mg/l; 72 h

OECD Test Guideline 201

Persistence and degradability

Biodegradability

Not readily biodegradable.

Bioaccumulative potential

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Partition coefficient: n-octanol/water

log Pow: -0.49

(calculated)

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

Mobility in soil

No information available.

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 1325
Proper shipping name FLAMMABLE SOLID, ORGANIC, N.O.S. (1,4-DIAZABICYCLO-OCTANE)
Class 4.1
Packing group II
Environmentally hazardous --

Air transport (IATA)

UN number UN 1325
Proper shipping name FLAMMABLE SOLID, ORGANIC, N.O.S. (1,4-DIAZABICYCLO-OCTANE)
Class 4.1
Packing group II
Environmentally hazardous --
Special precautions for user no

Sea transport (IMDG)

UN number UN 1325
Proper shipping name FLAMMABLE SOLID, ORGANIC, N.O.S. (1,4-DIAZABICYCLO-OCTANE)
Class 4.1
Packing group II
Environmentally hazardous --
Special precautions for user yes
EmS F-A S-G

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SECTION 15. Regulatory information

United States of America

OSHA Hazards

Flammable Solid

Harmful if swallowed.

Skin irritant

Eye 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.

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

US State Regulations

Massachusetts Right To Know

Remarks

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

Pennsylvania Right To Know

Ingredients

1,4-Diazabicyclo[2.2.2]octane

New Jersey Right To Know

Ingredients

1,4-Diazabicyclo[2.2.2]octane

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.

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Notification status

TSCA: All components of the product are listed in the 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.

H228	Flammable solid
H302	Harmful if swallowed.
H315	Causes skin irritation.
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.

Revision Date 08/21/2013

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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