

SAFETY DATA SHEET

Version 8.8
Revision Date 09/07/2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : 1,4-Diazabicyclo[2.2.2]octane for synthesis

Product Number : 8.03456
Catalogue No. : 803456
Brand : Millipore
CAS-No. : 280-57-9

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

Identified uses : Chemical for synthesis
Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

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

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable solids (Category 1), H228
Acute toxicity, Oral (Category 4), H302
Skin irritation (Category 2), H315
Serious eye damage (Category 1), H318

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

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H228 Flammable solid.
 H302 Harmful if swallowed.
 H315 Causes skin irritation.
 H318 Causes serious eye damage.

Precautionary Statements

P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
 P240 Ground/bond container and receiving equipment.
 P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.
 P264 Wash skin thoroughly after handling.
 P270 Do not eat, drink or smoke when using this product.
 P280 Wear protective gloves/ eye protection/ face protection.
 P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
 P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
 P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
 P332 + P313 If skin irritation occurs: Get medical advice/ attention.
 P362 Take off contaminated clothing and wash before reuse.
 P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
 P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula : C₆H₁₂N₂
 Molecular weight : 112.17 g/mol
 CAS-No. : 280-57-9
 EC-No. : 205-999-9

Component	Classification	Concentration
1,4-Diazabicyclo[2.2.2]octane	Flam. Sol. 1; Acute Tox. 4; Skin Irrit. 2; Eye Dam. 1; H228, H302, H315, H318	<= 100 %

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.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact

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

Water 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

Nature of decomposition products not known.

Combustible.

Fire may cause evolution of:

Ammonia, nitrogen oxides

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

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. 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

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. 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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

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

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Keep away from heat and sources of ignition.

Recommended storage temperature see product label.

Storage class

Storage class (TRGS 510): 4.1B: Flammable solid hazardous materials

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

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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). Tightly fitting safety goggles

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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested:KCL 741 Dermatril® L

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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested:KCL 741 Dermatril® L

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter type P2

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. required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

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) Appearance	Form: solid Color: white
b) Odor	Ammonia odor
c) Odor Threshold	No data available
d) pH	at 20 °C (68 °F)alkaline, Aqueous solution
e) Melting point/freezing point	Melting point: 158 °C (316 °F)
f) Initial boiling point and boiling range	173.4 °C 344.1 °F at 1,000 hPa
g) Flash point	62.2 °C (144.0 °F) - closed cup - ISO 1523
h) Evaporation rate	No data available
i) Flammability (solid, gas)	The substance or mixture is a flammable solid with the category 1. - Regulation (EC) No. 440/2008, Annex, A.10
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	0.43 hPa at 23 °C (73 °F) - OECD Test Guideline 104
l) Vapor density	No data available
m) Density	1.14 g/cm ³ at 28 °C (82 °F)
Relative density	No data available
n) Water solubility	610 g/l at 25 °C (77 °F) - soluble
o) Partition coefficient: n-octanol/water	log Pow: -0.49 at 20 °C (68 °F) - (calculated) - (Lit.), Bioaccumulation is not expected.
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

9.2 Other safety information

Bulk density	800 kg/m ³
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SECTION 10: Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.
A range from approx. 15 Kelvin below the flash point is to be rated as critical.
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.

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

Strong heating.

10.5 Incompatible materials

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 - 700 mg/kg

Remarks: (ECHA)

Symptoms: Possible damages:, mucosal irritations

LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg

Remarks: (ECHA)

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Irritations

Remarks: (ECHA)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye damage.

(OECD Test Guideline 405)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Millipore - 8.03456

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Metabolic activation: Metabolic activation
Method: OECD Test Guideline 471
Result: negative

Test Type: Chromosome aberration test
Species: Mouse
Cell type: Bone marrow

Method: OECD Test Guideline 474
Result: negative

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.
- 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.
- OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption:

Dizziness
Headache

Damage to:

Kidney

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	static test LC50 - <i>Cyprinus carpio</i> (Carp) - > 100 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - <i>Daphnia magna</i> (Water flea) - > 100 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test EC50 - <i>Pseudokirchneriella subcapitata</i> (green algae) - 110 mg/l - 72 h (OECD Test Guideline 201) static test NOEC - <i>Pseudokirchneriella subcapitata</i> (green algae) - 46 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC50 - <i>Pseudomonas putida</i> - 355.6 mg/l - 17 h Remarks: (ECHA)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 7 % - Not readily biodegradable. (OECD Test Guideline 301B)
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12.3 Bioaccumulative potential

Bioaccumulation	<i>Cyprinus carpio</i> (Carp) - 42 d - 1 mg/l(1,4-Diazabicyclo[2.2.2]octane) Bioconcentration factor (BCF): < 1.3 (OECD Test Guideline 305C)
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12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

DOT (US)

UN number: 1325 Class: 4.1 Packing group: II
Proper shipping name: Flammable solids, organic, n.o.s. (1,4-Diazabicyclo[2.2.2]octane)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 1325 Class: 4.1 Packing group: II EMS-No: F-A, S-G
Proper shipping name: FLAMMABLE SOLID, ORGANIC, N.O.S. (1,4-Diazabicyclo[2.2.2]octane)

IATA

UN number: 1325 Class: 4.1 Packing group: II
Proper shipping name: Flammable solid, organic, n.o.s. (1,4-Diazabicyclo[2.2.2]octane)

SECTION 15: Regulatory information

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

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.

US State Regulations

Massachusetts Right To Know

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

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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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