SAFETY DATA SHEET

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

Product Number: D27802
Brand: Sigma-Aldrich
CAS-No.: 280-57-9

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

Identified uses: Laboratory chemicals, Synthesis of substances

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

Precautionary statement(s)
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 + IF IN EYES: Rinse cautiously with water for several minutes.
P310 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.
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

<table>
<thead>
<tr>
<th>Synonyms</th>
<th>TED Triethylenediamine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>C₆H₁₂N₂</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>112.17 g/mol</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>280-57-9</td>
</tr>
<tr>
<td>EC-No.</td>
<td>205-999-9</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,4-Diazabicyclo[2.2.2]octane</td>
<td>Flam. Sol. 1; Acute Tox. 4; Skin Irrit. 2; Eye Dam. 1; H228, H302, H315, H318</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

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.
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. strongly hygroscopic Air and moisture sensitive. Handle and store under inert gas.

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 EN374 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

- **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**
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: crystalline
  - 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/range: 156 - 159 °C (313 - 318 °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
   1.02 g/mL at 25 °C (77 °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
   No data available

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
Violent reactions possible with:
- mineral acids
- Strong oxidizing agents
- peroxi compounds
- iron/iron-containing compounds
- acids
Risk of explosion with:
- hydrogen peroxide

10.4 Conditions to avoid
- Exposure to moisture.
- Strong heating.

10.5 Incompatible materials
- Aluminum, Iron, Copper, Zinc

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
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

RTECS: HM0354200
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 - *Cyprinus carpio* (Carp) - > 100 mg/l - 96 h
Toxicity to daphnia and other aquatic invertebrates
static test EC50 - Daphnia magna (Water flea) - > 100 mg/l - 48 h
(OED Test Guideline 202)

Toxicity to algae
static test EC50 - Pseudokirchneriella subcapitata (green algae) - 110 mg/l - 72 h
(OECD Test Guideline 201)
static test NOEC - Pseudokirchneriella subcapitata (green algae) - 46 mg/l - 72 h
(OECD Test Guideline 201)

Toxicity to bacteria
static test EC50 - Pseudomonas putida - 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)

12.3 Bioaccumulative potential
Bioaccumulation
Cyprinus carpio (Carp) - 42 d
- 1 mg/l(1,4-Diazabicyclo[2.2.2]octane)
Bioconcentration factor (BCF): < 1.3
(OECD Test Guideline 305C)

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

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

**SARA 313 Components**
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 311/312 Hazards**
Fire Hazard, Acute Health Hazard

**Massachusetts Right To Know Components**
No components are subject to the Massachusetts Right to Know Act.

SECTION 16: Other information

**Further information**
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact misbranding@sial.com.

Version: 6.9  Revision Date: 06/16/2023  Print Date: 01/06/2024