1. PRODUCT AND COMPANY IDENTIFICATION

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, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO  63103
USA
Telephone: +1 800-325-5832
Fax: +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone #: (314) 776-6555

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
Eye irritation (Category 2A), H319
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
Acute aquatic toxicity (Category 3), H402
Chronic aquatic toxicity (Category 3), H412

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.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation.
H412 Harmful to aquatic life with long lasting effects.

Precautionary statement(s)
P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

<table>
<thead>
<tr>
<th>Synonyms</th>
<th>TED Triethylenediamine</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Formula</th>
<th>C₆H₁₂N₂</th>
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</thead>
<tbody>
<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>
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</table>

<table>
<thead>
<tr>
<th>Hazardous components</th>
</tr>
</thead>
<tbody>
<tr>
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</tr>
<tr>
<td>1,4-Diazabicyclooctane</td>
</tr>
</tbody>
</table>

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

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice
Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.
In case of skin contact
Wash off with soap and plenty of water. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

5. FIREFIGHTING MEASURES

5.1 Extinguishing media
Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
Carbon oxides, nitrogen oxides (NOx)
Nature of decomposition products not known.
Carbon oxides, nitrogen oxides (NOx)

5.3 Advice for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Avoid breathing dust.
For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Sweep up and shovel. Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal. Contain spillage, pick up with an electrically protected vacuum cleaner or by wet-brushing and transfer to a container for disposal according to local regulations (see section 13).

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Store in cool place. Keep container tightly closed in a dry and well-ventilated place.
strongly hygroscopic Air and moisture sensitive. Handle and store under inert gas.

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated
8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters
Contents no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection
Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection
Complete suit protecting against chemicals, Flame retardant antistatic protective clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance Form: solid
b) Odour no data available
c) Odour Threshold no data available
d) pH no data available
e) Melting point/freezing point  
   Melting point/range: 156 - 159 °C (313 - 318 °F)

f) Initial boiling point and boiling range  
   174 °C (345 °F)

g) Flash point  
   62 °C (144 °F) - closed cup

h) Evaporation rate  
   no data available

i) Flammability (solid, gas)  
   The substance or mixture is a flammable solid with the category 1.

j) Upper/lower flammability or explosive limits  
   no data available

k) Vapour pressure  
   3.9 hPa (2.9 mmHg) at 50 °C (122 °F)

l) Vapour density  
   no data available

m) Relative density  
   1.02 g/mL at 25 °C (77 °F)

n) Water solubility  
   soluble

o) Partition coefficient: n-octanol/water  
   no data available

p) Auto-ignition temperature  
   no data available

q) Decomposition temperature  
   no data available

r) Viscosity  
   no data available

s) Explosive properties  
   no data available

t) Oxidizing properties  
   no data available

9.2 Other safety information
   no data available

10. STABILITY AND REACTIVITY

10.1 Reactivity
   no data available

10.2 Chemical stability
   Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
   no data available

10.4 Conditions to avoid
   Exposure to moisture, heat, flames and sparks. Extremes of temperature and direct sunlight.

10.5 Incompatible materials
   Strong oxidizing agents, Strong acids

10.6 Hazardous decomposition products
   Other decomposition products - no data available
   In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

   Acute toxicity
   LD50 Oral - rat - 1,700 mg/kg
   Dermal: no data available
no data available

**Skin corrosion/irritation**

Serious eye damage/eye irritation

Eyes - rabbit

Result: Eye irritation

**Respiratory or skin sensitisation**

no data available

**Germ cell mutagenicity**

no data available

**Carcinogenicity**

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component 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 identified as a carcinogen or potential carcinogen by OSHA.

**Reproductive toxicity**

no data available

no data available

**Specific target organ toxicity - single exposure**

Inhalation - May cause respiratory irritation.

**Specific target organ toxicity - repeated exposure**

no data available

**Aspiration hazard**

no data available

**Additional Information**

RTECS: HM0354200

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

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12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish

LC50 - Pimephales promelas (fathead minnow) - 1,730.0 mg/l - 96.0 h

Toxicity to daphnia and other aquatic invertebrates

EC50 - Daphnia magna (Water flea) - 92 mg/l - 48 h

12.2 Persistence and degradability

Biodegradability

Result: 7 % - Not readily biodegradable.

12.3 Bioaccumulative potential

no data available

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 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

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-Diazabicyclooctane)
Marine pollutant: No
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-Diazabicyclooctane)
Marine pollutant: No

IATA
UN number: 1325 Class: 4.1 Packing group: II
Proper shipping name: Flammable solid, organic, n.o.s. (1,4-Diazabicyclooctane)

15. REGULATORY INFORMATION

SARA 302 Components
SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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

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

Pennsylvania Right To Know Components

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New Jersey Right To Know Components

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California Prop. 65 Components
This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

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

Acute Tox. Acute toxicity
Aquatic Acute Acute aquatic toxicity
Aquatic Chronic  Chronic aquatic toxicity
Eye Irrit.  Eye irritation
Flam. Sol.  Flammable solids
H228  Flammable solid.
H302  Harmful if swallowed.
H315  Causes skin irritation.
H319  Causes serious eye irritation.
H335  May cause respiratory irritation.

HMIS Rating
Health hazard:  2
Chronic Health Hazard:  
Flammability:  3
Physical Hazard  3

NFPA Rating
Health hazard:  2
Fire Hazard:  3
Reactivity Hazard:  3

Further information
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Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 5.3  Revision Date: 06/17/2014  Print Date: 06/20/2016