SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name: 1,3,5-Trioxane

Product Number: T81108
Brand: Aldrich
Index-No.: 605-002-00-0
CAS-No.: 110-88-3

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
Reproductive toxicity (Category 2), H361
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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.
H335  May cause respiratory irritation.
H361  Suspected of damaging fertility or the unborn child.

Precautionary statement(s)
P201  Obtain special instructions before use.
P202  Do not handle until all safety precautions have been read and understood.
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.
P261  Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P271  Use only outdoors or in a well-ventilated area.
P280  Wear protective gloves/ protective clothing/ eye protection/ face protection.
P304 + P340  IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P308 + P313  IF exposed or concerned: Get medical advice/ attention.
P370 + P378  In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P403 + P233  Store in a well-ventilated place. Keep container tightly closed.
P405  Store locked up.
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 : C₃H₆O₃
Molecular weight : 90.08 g/mol
CAS-No. : 110-88-3
EC-No. : 203-812-5
Index-No. : 605-002-00-0

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,3,5-Trioxane</td>
<td>Flam. Sol. 1; Repr. 2; STOT SE 3; H228, H361, H335</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. Call in physician.

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

In case of eye contact
After eye contact: rinse out with plenty of water. 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

Unsuitable extinguishing media
For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Vapors are heavier than air and may spread along floors.

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
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
Change contaminated clothing. Preventive skin protection recommended. Wash hands 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.
Exposure to moisture.

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
Change contaminated clothing. Preventive skin protection recommended. Wash hands 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). Safety glasses

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 EC 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**
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: colorless

- **b)** Odor
  - No data available

- **c)** Odor Threshold
  - No data available

- **d)** pH
  - No data available

- **e)** Melting point/freezing point
  - Melting point/range: 59 - 62 °C (138 - 144 °F)

- **f)** Initial boiling point
  - 112 - 115 °C 234 - 239 °F at 1013 hPa

- **g)** Flash point
  - 45 °C (113 °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
  - Upper explosion limit: 29 %(V)
  - Lower explosion limit: 3.6 %(V)

- **k)** Vapor pressure
  - 11 hPa at 20 °C (68 °F)

- **l)** Vapor density
  - No data available
m) Density
   1.38 g/cm³ at 20 °C (68 °F) - OECD Test Guideline 109
   Relative density
   No data available

n) Water solubility
   172 g/l at 20 °C (68 °F)

o) Partition coefficient:
   n-octanol/water
   log Pow: -0.5 at 25 °C (77 °F)

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
   No data available

9.2 Other safety information
   No data available

SECTION 10: Stability and reactivity

10.1 Reactivity
   No data available

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
   No information available

10.5 Incompatible materials
   Strong oxidizing agents, Acrylonitrile, Hydrogen peroxide, Lead

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 - > 2,000 mg/kg
   LC₅₀ Inhalation - Rat - male and female - 4 h - > 39.2 mg/l - dust/mist
   LD₅₀ Dermal - Rabbit - > 3,980 mg/kg
   Remarks: (Lit.)

   Skin corrosion/irritation
   Skin - Rabbit
   Result: No skin irritation
(OECD Test Guideline 404)

**Serious eye damage/eye irritation**
Eyes - Rabbit
Result: No eye irritation

(OECD Test Guideline 405)
Eyes - Rabbit
Result: No eye irritation
Remarks: slight irritation

**Respiratory or skin sensitization**
Maximization Test - Guinea pig
Did not cause sensitization on laboratory animals.

**Germ cell mutagenicity**
Test Type: Ames test
Test system: Chinese hamster lung cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative
Remarks: (Lit.)

Test Type: Chromosome aberration test in vitro
Test system: fibroblast
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 473
Result: negative

Test Type: Micronucleus test
Result: negative
Remarks: (Lit.)

Species: Rat

Application Route: Gavage
Method: OECD Test Guideline 486
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.

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.

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**
Suspected of damaging the unborn child.
Suspected human reproductive toxicant
Specific target organ toxicity - single exposure
May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

11.2 Additional Information
RTECS: YK0350000
burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity
Toxicity to fish static test LC50 - Leuciscus idus (Golden orfe) - ca. 4,000 mg/l - 96 h
Toxicity to daphnia and other aquatic invertebrates static test EC50 - Daphnia magna (Water flea) - > 1,000 mg/l - 48 h
Toxicity to algae static test EC50 - Desmodesmus subspicatus (green algae) - > 500 mg/l - 72 h

12.2 Persistence and degradability
Biodegradability aerobic - Exposure time 28 d
Result: 0 - 10 % - Not rapidly biodegradable (OECD Test Guideline 301C)

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 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. (1,3,5-Trioxane)
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. (1,3,5-Trioxane)

IATA
UN number: 1325  Class: 4.1  Packing group: II
Proper shipping name: Flammable solid, organic, n.o.s. (1,3,5-Trioxane)

SECTION 15: Regulatory information

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

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, Chronic Health Hazard

Massachusetts Right To Know Components

<table>
<thead>
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Pennsylvania Right To Know Components

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New Jersey Right To Know Components

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California Prop. 65 Components

Aldrich - T81108
This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

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.

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