SAFETY DATA SHEET

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

1.1 Product identifiers

Product name: 1,4-Dioxane-d₈

Product Number: 186406
Brand: Aldrich
Index-No.: 603-024-00-5
CAS-No.: 17647-74-4

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 liquids (Category 2), H225
Eye irritation (Category 2A), H319
Carcinogenicity (Category 1B), H350
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

Aldrich - 186406
Signal Word: Danger

Hazard statement(s)
- H225: Highly flammable liquid and vapor.
- H319: Causes serious eye irritation.
- H335: May cause respiratory irritation.
- H350: May cause cancer.

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.
- P233: Keep container tightly closed.
- P240: Ground/bond container and receiving equipment.
- P241: Use explosion-proof electrical/ ventilating/ lighting/ equipment.
- P242: Use only non-sparking tools.
- P243: Take precautionary measures against static discharge.
- P261: Avoid breathing mist or vapors.
- P264: Wash skin thoroughly after handling.
- P271: Use only outdoors or in a well-ventilated area.
- P280: Wear protective gloves/ protective clothing/ eye protection/ face protection.
- P303 + P361 + P353: IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
- P304 + P340 + P312: IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
- P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
- P308 + P313: IF exposed or concerned: Get medical advice/ attention.
- P337 + P313: If eye irritation persists: Get medical advice/ attention.
- P370 + P378: In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
- P403 + P233: Store in a well-ventilated place. Keep container tightly closed.
- P403 + P235: Store in a well-ventilated place. Keep cool.
- 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
May form explosive peroxides.
Repeated exposure may cause skin dryness or cracking.

SECTION 3: Composition/information on ingredients

3.1 Substances

<table>
<thead>
<tr>
<th>Synonyms</th>
<th>Octadeuterodioxane</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>p-Dioxane-d8</td>
</tr>
</tbody>
</table>

| Formula | C₄D₈O₂ |

Aldrich - 186406
Molecular weight : 96.15 g/mol
CAS-No. : 17647-74-4
EC-No. : 241-628-7
Index-No. : 603-024-00-5

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Octadeuterodioxane</td>
<td>Flam. Liq. 2; Eye Irrit. 2A; Carc. 1B; STOT SE 3; H225, H319, H350, 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

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**
Carbon oxides
Combustible.
Pay attention to flashback.
Vapors are heavier than air and may spread along floors.
Development of hazardous combustion gases or vapours possible in the event of fire.
Forms explosive mixtures with air at ambient temperatures.

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. 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: Do not breathe vapors, aerosols. 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 carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 **Reference to other sections**
For disposal see section 13.

**SECTION 7: Handling and storage**

7.1 **Precautions for safe handling**

**Advice on safe handling**
Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

**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**
Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Test for peroxide formation periodically and before distillation.

**Storage class**
Storage class (TRGS 510): 3: Flammable liquids

**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

<table>
<thead>
<tr>
<th>Ingredients with workplace control parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Component</td>
</tr>
<tr>
<td>Octadeuterodioxane</td>
</tr>
<tr>
<td>Remarks</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>C</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>TWA</td>
</tr>
<tr>
<td>Skin designation</td>
</tr>
</tbody>
</table>

#### 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). Safety glasses

**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: butyl-rubber
Minimum layer thickness: 0.7 mm
Break through time: 480 min
Material tested: Butoject® (KCL 898)

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).

Splash contact
Material: Viton®
Minimum layer thickness: 0.7 mm
Break through time: 120 min
Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

**Body Protection**
Flame retardant antistatic protective clothing.

**Respiratory protection**
Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

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 vapours/aerosols 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.

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**SECTION 9: Physical and chemical properties**

9.1 **Information on basic physical and chemical properties**

<table>
<thead>
<tr>
<th>a) Appearance</th>
<th>Form: clear, liquid</th>
<th>Color: colorless</th>
</tr>
</thead>
<tbody>
<tr>
<td>b) Odor</td>
<td>No data available</td>
<td></td>
</tr>
<tr>
<td>c) Odor Threshold</td>
<td>No data available</td>
<td></td>
</tr>
<tr>
<td>d) pH</td>
<td>No data available</td>
<td></td>
</tr>
<tr>
<td>e) Melting point/freezing point</td>
<td>No data available</td>
<td></td>
</tr>
<tr>
<td>f) Initial boiling point and boiling range</td>
<td>99 °C 210 °F - lit.</td>
<td></td>
</tr>
<tr>
<td>g) Flash point</td>
<td>5 °C (41 °F) - closed cup</td>
<td></td>
</tr>
<tr>
<td>h) Evaporation rate</td>
<td>No data available</td>
<td></td>
</tr>
</tbody>
</table>

Aldrich - 186406
i) Flammability (solid, gas) No data available
j) Upper/lower flammability or explosive limits No data available
k) Vapor pressure No data available
l) Vapor density No data available
m) Density 1.129 g/cm³ at 25 °C (77 °F) - lit.
   Relative density No data available
n) Water solubility No data available
o) Partition coefficient: n-octanol/water No data available
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
Formation of peroxides possible.
Vapors may form explosive mixture with air.

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

10.3 Possibility of hazardous reactions
Risk of explosion with:
triethylaluminium
lithium aluminium hydride
Triethylamine
Boranes
silver perchlorate
Oxygen
Nitric acid
with
perchloric acid
Raney-nickel
with
Hydrogen
Risk of ignition or formation of inflammable gases or vapours with:
fire-promoting substances
Exothermic reaction with:
Oxidizing agents
Sulfur trioxide
acids

10.4 Conditions to avoid
Avoid moisture. Heat.
Warming.
Moisture.

10.5 Incompatible materials
No data available

10.6 Hazardous decomposition products
Peroxides
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - male and female - 5,150 mg/kg
(OECD Test Guideline 401)
Remarks: The value is given in analogy to the following substances: 1,4-Dioxane
Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:; damage of respiratory tract, Lung edema
LD50 Dermal - Rabbit - 7,378 mg/kg
Remarks: (RTECS)
The value is given in analogy to the following substances: 1,4-Dioxane

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 20 h
Remarks: (IUCLID)
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
The value is given in analogy to the following substances: 1,4-Dioxane

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Eye irritation
(OECD Test Guideline 405)
Remarks: The value is given in analogy to the following substances: 1,4-Dioxane

Respiratory or skin sensitization
Maximization Test - Guinea pig
Result: negative
Remarks: The value is given in analogy to the following substances: 1,4-Dioxane

Germ cell mutagenicity
Test Type: Ames test
Test system: Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative
Remarks: The value is given in analogy to the following substances: 1,4-Dioxane

Test Type: In vitro mammalian cell gene mutation test
Test system: Chinese hamster ovary cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative
Remarks: The value is given in analogy to the following substances: 1,4-Dioxane

Test Type: Chromosome aberration test in vitro
Test system: Chinese hamster ovary cells
Metabolic activation: with and without metabolic activation
Result: negative
Remarks: (ECHA) The value is given in analogy to the following substances: 1,4-Dioxane


carcinogenicity
Presumed to have carcinogenic potential for humans
IARC: 2B - Group 2B: Possibly carcinogenic to humans (Octadeuterodioxane)
NTP: RAHC - Reasonably anticipated to be a human carcinogen (Octadeuterodioxane)
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
May cause respiratory irritation. - Respiratory system
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
The value is given in analogy to the following substances: 1,4-Dioxane

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

11.2 Additional Information
Repeated dose toxicity - Rat - male - Oral - 716 Days - NOAEL (No observed adverse effect level) - 9.6 mg/kg
Remarks: (ECHA) The value is given in analogy to the following substances: 1,4-Dioxane
Nausea, Vomiting, Weakness, Dizziness, Vertigo, Headache, Sweating, loss of appetite, Kidney injury may occur., Liver injury may occur.
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.
The substance has delayed effects.

After absorption:

Headache
Dizziness
Nausea
Vomiting

Absorption can result in damage to:

Liver
Kidney

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Stomach - Irregularities - Based on Human Evidence
Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to daphnia and other aquatic invertebrates

semi-static test EC50 - Daphnia magna (Water flea) - > 1,000 mg/l - 48 h
(OECD Test Guideline 202)
Remarks: The value is given in analogy to the following substances: 1,4-Dioxane

Toxicity to algae

static test ErC50 - Pseudokirchneriella subcapitata (green algae) - > 1,000 mg/l - 72 h
(OECD Test Guideline 201)
Remarks: The value is given in analogy to the following substances: 1,4-Dioxane

Toxicity to fish (Chronic toxicity)

flow-through test NOEC - Pimephales promelas (fathead minnow) - > 103 mg/l - 32 d
Remarks: (ECHA)
The value is given in analogy to the following substances: 1,4-Dioxane
12.2 Persistence and degradability

Biodegradability
- Aerobic - Exposure time 29 d
- Result: < 10% - Not readily biodegradable.

Remarks: The value is given in analogy to the following substances: 1,4-Dioxane

12.3 Bioaccumulative potential

Bioaccumulation
- Cyprinus carpio (Carp) - 10 mg/l (Octadeuterodioxane)

Bioconcentration factor (BCF): 0.3 - 0.7

Remarks: The value is given in analogy to the following substances: 1,4-Dioxane

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

Forms toxic mixtures in water, dilution measures notwithstanding. Discharge into the environment must be avoided.

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: 1165
- Class: 3
- Packing group: II
- Proper shipping name: Dioxane

Aldrich - 186406
Reportable Quantity (RQ): 100 lbs
Poison Inhalation Hazard: No

**IMDG**
- UN number: 1165  Class: 3  Packing group: II  EMS-No: F-E, S-D
- Proper shipping name: DIOXANE

**IATA**
- UN number: 1165  Class: 3  Packing group: II
- Proper shipping name: Dioxane

### SECTION 15: Regulatory information

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

**SARA 313 Components**
The following components are subject to reporting levels established by SARA Title III, Section 313:

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
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<tbody>
<tr>
<td>Octadeuterodioxane</td>
<td>17647-74-4</td>
<td>2007-07-01</td>
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</tbody>
</table>

**SARA 311/312 Hazards**
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

<table>
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**Pennsylvania Right To Know Components**

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</tbody>
</table>

**California Prop. 65 Components**
, which is/are known to the State of California to cause cancer. For more information go to www.P65Warnings.ca.gov.Octadeuterodioxane
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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Details in analogy to the undeuterated compound.

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