



SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 7.2

Revision Date 30.12.2023

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

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

REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

CAS-No. : 17647-74-4

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

Identified uses : Laboratory chemicals, Manufacture of substances

1.3

CHEMIKART

1.4 Emergency telephone

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Flammable liquids, (Category 2) H225: Highly flammable liquid and vapor.

Eye irritation, (Category 2) H319: Causes serious eye irritation.

Carcinogenicity, (Category 1B) H350: May cause cancer.

Specific target organ toxicity -
single exposure, (Category 3),
Respiratory system

H335: May cause respiratory irritation.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal Word	Danger
Hazard Statements	
H225	Highly flammable liquid and vapor.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H350	May cause cancer.
Precautionary Statements	
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233	Keep container tightly closed.
P240	Ground and bond container and receiving equipment.
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.
Supplemental Hazard information (EU)	
EUH019	May form explosive peroxides.
EUH066	Repeated exposure may cause skin dryness or cracking.
	Restricted to professional users.

Reduced Labeling (<= 125 ml)

Pictogram

Signal Word	Danger
Hazard Statements	
H350	May cause cancer.
Precautionary Statements	
P202	Do not handle until all safety precautions have been read and understood.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
Supplemental Hazard information (EU)	
EUH019	May form explosive peroxides.
EUH066	Repeated exposure may cause skin dryness or cracking.

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Toxicological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : Octadeuterodioxane
p-Dioxane-d8

Formula : C₄D₈O₂
Molecular weight : 96,15 g/mol
CAS-No. : 17647-74-4
EC-No. : 241-628-7
Index-No. : 603-024-00-5

Component	Classification	Concentration
Octadeuterodioxane Included in the Candidate List of Substances of Very High Concern (SVHC) according to Regulation (EC) No. 1907/2006 (REACH)		
CAS-No. 17647-74-4 EC-No. 241-628-7	Flam. Liq. 2; Eye Irrit. 2; Carc. 1B; STOT SE 3; H225, H319, H350, H335	<= 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. 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. Chemisorb®). 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

Ingredients with workplace control parameters

8.2 Exposure controls

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 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: 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 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: 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.

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) Physical state | clear, liquid |
| b) Color | colorless |
| c) Odor | No data available |
| d) Melting point/freezing point | No data available |
| e) Initial boiling point and boiling range | 99 °C - lit. |
| f) Flammability (solid, gas) | No data available |
| g) Upper/lower flammability or explosive limits | No data available |
| h) Flash point | 5 °C - closed cup |
| i) Autoignition temperature | No data available |
| j) Decomposition temperature | No data available |

- | | |
|--|--|
| k) pH | No data available |
| l) Viscosity | Viscosity, kinematic: No data available
Viscosity, dynamic: No data available |
| m) Water solubility | No data available |
| n) Partition coefficient:
n-octanol/water | No data available |
| o) Vapor pressure | No data available |
| p) Density | 1,129 g/cm ³ at 25 °C - lit. |
| Relative density | No data available |
| q) Relative vapor
density | No data available |
| r) Particle
characteristics | 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

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(Regulation (EC) No. 440/2008, Annex, B.6)

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

Test Type: unscheduled DNA synthesis assay

Species: Rat

Cell type: Liver cells

Application Route: Oral

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

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

Endocrine disrupting properties

Product:

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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.

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
Toxicity to daphnia and other aquatic invertebrates(Chronic	NOEC - Daphnia magna (Water flea) - 1.000 mg/l - 21 d (OECD Test Guideline 211) Remarks: The value is given in analogy to the following substances:

toxicity)

1,4-Dioxane

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 29 d
Result: < 10 % - Not readily biodegradable.
(OECD Test Guideline 301F)
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
(OECD Test Guideline 305C)

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

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Endocrine disrupting properties

Product:
Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1165

IMDG: 1165

IATA: 1165

14.2 UN proper shipping name

ADR/RID: DIOXANE

IMDG: DIOXANE

IATA: Dioxane

14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA: 3

14.4 Packaging group

ADR/RID: II

IMDG: II

IATA: II

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

14.6 Special precautions for user

Tunnel restriction code : (D/E)

Further information : No data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

Authorisations and/or restrictions on use

REACH - Candidate List of Substances of Very High Concern for Authorisation (Article 59). : Octadeuterodioxane

REACH - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles (Annex XVII) : Octadeuterodioxane

National legislation

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances. P5c FLAMMABLE LIQUIDS

Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of H-Statements

H225	Highly flammable liquid and vapor.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H350	May cause cancer.
EUH019	May form explosive peroxides.
EUH066	Repeated exposure may cause skin dryness or cracking.

Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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

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Details in analogy to the undeuterated compound.

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