

## SAFETY DATA SHEET

Version 6.4  
Revision Date 04/21/2021  
Print Date 02/11/2022

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 1,4-Dioxane-dg

Product Number : 4M4829-U  
Brand : Supelco  
Index-No. : 603-001-00-X  
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  
Acute toxicity, Oral (Category 3), H301  
Acute toxicity, Inhalation (Category 3), H331  
Acute toxicity, Dermal (Category 3), H311  
Carcinogenicity (Category 2), H351  
Specific target organ toxicity - single exposure (Category 1), Eyes, Central nervous system,  
H370

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

**2.2 GHS Label elements, including precautionary statements**

Pictogram



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Signal word	Danger
Hazard statement(s)	
H225	Highly flammable liquid and vapor.
H301 + H311 + H331	Toxic if swallowed, in contact with skin or if inhaled.
H351	Suspected of causing cancer.
H370	Causes damage to organs (Eyes, Central nervous system).
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.
P260	Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P311	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.
P307 + P311	IF exposed: Call a POISON CENTER or doctor/ physician.
P362	Take off contaminated clothing and wash before reuse.
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 - none

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## SECTION 3: Composition/information on ingredients

### 3.2 Mixtures

Synonyms	:	Octadeuterodioxane p-Dioxane-d8
Formula	:	C <sub>4</sub> D <sub>8</sub> O <sub>2</sub> C <sub>4</sub> D <sub>8</sub> O <sub>2</sub>
Molecular weight	:	96.15 g/mol

Component	Classification	Concentration
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<b>Methanol</b>			
CAS-No.	67-56-1	Flam. Liq. 2; Acute Tox. 3;	≥ 90 - ≤ 100 %
EC-No.	200-659-6	STOT SE 1; H225, H301,	
Index-No.	603-001-00-X	H331, H311, H370	
Registration number	01-2119433307-44-XXXX	Concentration limits: ≥ 10 %: STOT SE 1, H370; 3 - < 10 %: STOT SE 2, H371;	
<b>Octadeuterodioxane</b>			
CAS-No.	17647-74-4	Flam. Liq. 2; Eye Irrit. 2A;	≥ 0.1 - < 1 %
EC-No.	241-628-7	Carc. 2; STOT SE 3; H225,	
Index-No.	603-024-00-5	H319, H351, H335 Concentration limits: ≥ 20 %: STOT SE 3, H335;	

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

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

#### In case of skin contact

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

#### In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

#### If swallowed

After swallowing: fresh air. Make victim drink ethanol (e.g. 1 drinking glass of a 40% alcoholic beverage). Call a doctor immediately (mention methanol ingestion). Only in exceptional cases, if no medical care is available within one hour, induce vomiting (only in fully conscious persons) and make victim drink ethanol again (approx. 0.3 ml of a 40% alcoholic beverage/kg body weight/hour).

### 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

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Water Foam Carbon dioxide (CO<sub>2</sub>) 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.

Risk of dust explosion.

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.

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## 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.

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## 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.

### Storage stability

Recommended storage temperature

2 - 8 °C

hygroscopic Store under inert gas.

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

Component	CAS-No.	Value	Control parameters	Basis
Methanol	67-56-1	TWA	200 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Danger of cutaneous absorption		
		STEL	250 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Danger of cutaneous absorption		
		TWA	200 ppm 260 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		ST	250 ppm 325 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	200 ppm 260 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		STEL	250 ppm 325 mg/m <sup>3</sup>	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation		
		TWA	200 ppm 260 mg/m <sup>3</sup>	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation		

		C	1,000 ppm	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		PEL	200 ppm 260 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		STEL	250 ppm 325 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
Octadeuterodioxane	17647-74-4	TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption		
		TWA	25 ppm 90 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation		
		TWA	100 ppm 360 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Skin designation		
		C	1 ppm 3.6 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential Occupational Carcinogen		
		PEL	0.28 ppm 1 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

#### Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Methanol	67-56-1	Methanol	15 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			

## 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

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: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: 480 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 30 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, 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 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

- |                                 |                                       |
|---------------------------------|---------------------------------------|
| a) Appearance                   | Form: liquid                          |
| b) Odor                         | No data available                     |
| c) Odor Threshold               | No data available                     |
| d) pH                           | No data available                     |
| e) Melting point/freezing point | Melting point/range: -98 °C (-144 °F) |
| f) Initial boiling point        | 99 °C 210 °F - lit.                   |

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	and boiling range	
g)	Flash point	10 °C (50 °F) - closed cup
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	Upper explosion limit: 36.5 %(V) Lower explosion limit: 6 %(V)
k)	Vapor pressure	133 hPa at 25 °C (77 °F)
l)	Vapor density	No data available
m)	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	No data available

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

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

No data available

### 10.4 Conditions to avoid

Warming.

### 10.5 Incompatible materials

Acids, Oxidizing agents, Alkali metals, Acid chlorides, Acid anhydrides, Reducing agents, Oxygen, Halogens

### 10.6 Hazardous decomposition products

In the event of fire: see section 5



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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Mixture

##### Acute toxicity

Acute toxicity estimate Oral - 100.1 mg/kg  
(Calculation method)

Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l  
(Calculation method)

Acute toxicity estimate Dermal - 300.1 mg/kg  
(Calculation method)  
No data available

##### Skin corrosion/irritation

No data available

##### Serious eye damage/eye irritation

No data available

##### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

No data available

#### Carcinogenicity

Evidence of a carcinogenic effect.

IARC: 2B - Group 2B: Possibly carcinogenic to humans (Octadeuterodioxane)

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

No data available

#### Specific target organ toxicity - single exposure

Remarks: No data available Mixture causes damage to organs. - Eyes, Central nervous system

### **Specific target organ toxicity - repeated exposure**

No data available

### **Aspiration hazard**

No data available

## **11.2 Additional Information**

Not available

Methyl alcohol may be fatal or cause blindness if swallowed., Cannot be made non-poisonous., Effects due to ingestion may include:, Nausea, Dizziness, Gastrointestinal disturbance, Weakness, Confusion., Drowsiness, Unconsciousness, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Central nervous system - Breathing difficulties - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

## **Components**

### **Methanol**

#### **Acute toxicity**

Acute toxicity estimate Oral - 100.1 mg/kg  
(Expert judgment)

Symptoms: Nausea, Vomiting

Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l  
(Expert judgment)

Symptoms: Irritation symptoms in the respiratory tract.

Acute toxicity estimate Dermal - 300.1 mg/kg  
(Expert judgment)

#### **Skin corrosion/irritation**

Skin - Rabbit

Result: No skin irritation

Remarks:

(ECHA)

Drying-out effect resulting in rough and chapped skin.

#### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: No eye irritation

Remarks:

(ECHA)

#### **Respiratory or skin sensitization**

Sensitisation test: - Guinea pig

Result: negative

(OECD Test Guideline 406)

#### **Germ cell mutagenicity**

Based on available data the classification criteria are not met.

Ames test  
Salmonella typhimurium  
Result: negative  
In vitro mammalian cell gene mutation test  
Chinese hamster lung cells  
Result: negative  
OECD Test Guideline 474  
Mouse - male and female - Bone marrow  
Result: negative

**Carcinogenicity**

Did not show carcinogenic effects in animal experiments.

**Reproductive toxicity**

Based on available data the classification criteria are not met.

**Specific target organ toxicity - single exposure**

Causes damage to organs. - Eyes, Central nervous system

Remarks:

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Acute oral toxicity - Nausea, Vomiting

Acute inhalation toxicity - Irritation symptoms in the respiratory tract.

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Octadeuterodioxane**

**Acute toxicity**

No data available

Inhalation: No data available

Dermal: No data available

No data available

**Skin corrosion/irritation**

No data available

**Serious eye damage/eye irritation**

No data available

**Respiratory or skin sensitization**

No data available

**Germ cell mutagenicity**

No data available

**Carcinogenicity**

Carcinogen

Limited evidence of carcinogenicity in animal studies

**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

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**SECTION 12: Ecological information****12.1 Toxicity****Mixture**

No data available

**12.2 Persistence and degradability**

No data available

**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**

No data available

**Components****Methanol**

Toxicity to fish	flow-through test LC50 - <i>Lepomis macrochirus</i> (Bluegill) - 15,400.0 mg/l - 96 h (US-EPA)
Toxicity to daphnia and other aquatic invertebrates	semi-static test EC50 - <i>Daphnia magna</i> (Water flea) - 18,260 mg/l - 96 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - <i>Pseudokirchneriella subcapitata</i> (green algae) - ca. 22,000.0 mg/l - 96 h (OECD Test Guideline 201)
Toxicity to bacteria	static test IC50 - activated sludge - > 1,000 mg/l - 3 h (OECD Test Guideline 209)

**Octadeuterodioxane**

No data available

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**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. See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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**SECTION 14: Transport information****DOT (US)**

UN number: 1230 Class: 3 Packing group: II  
Proper shipping name: MethanolSOLUTION

Reportable Quantity (RQ): 5000 lbs  
Poison Inhalation Hazard: No

**IMDG**

UN number: 1230 Class: 3 (6.1) Packing group: II EMS-No: F-E, S-D  
Proper shipping name: METHANOLSOLUTION

**IATA**

UN number: 1230 Class: 3 (6.1) Packing group: II  
Proper shipping name: MethanolSOLUTION

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**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:

	CAS-No.	Revision Date
Methanol	67-56-1	2007-07-01
Octadeuterodioxane	17647-74-4	2007-03-01

**SARA 311/312 Hazards**

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

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

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**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](http://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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