

## SAFETY DATA SHEET

Version 4.6  
Revision Date 05/27/2016  
Print Date 09/22/2019

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1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : 2-Propanol-1,1,1,3,3,3-d<sub>6</sub>

Product Number : 392898

Brand : Aldrich

CAS-No. : 3976-29-2

## 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  
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 # : +1-703-527-3887 (CHEMTREC)

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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

Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336

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)

H225

Highly flammable liquid and vapour.

H319

Causes serious eye irritation.

H336

May cause drowsiness or dizziness.

Precautionary statement(s)

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 dust/ fume/ gas/ mist/ vapours/ spray.

|                    |                                                                                                                                  |
|--------------------|----------------------------------------------------------------------------------------------------------------------------------|
| P264               | Wash skin thoroughly after handling.                                                                                             |
| P271               | Use only outdoors or in a well-ventilated area.                                                                                  |
| P280               | Wear protective gloves/ eye protection/ face protection.                                                                         |
| P303 + P361 + P353 | IF ON SKIN (or hair): Take off immediately all contaminated clothing.<br>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. |
| 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 - none

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

|                           |                                                                                                                                                                                    |
|---------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Chemical characterization | : Isotopically labeled                                                                                                                                                             |
| Synonyms                  | : Isopropanol-1,1,1,3,3,3-d <sub>6</sub><br>Isopropanol-1,1,1,3,3,3-d <sub>6</sub><br>Isopropyl-1,1,1,3,3,3-d <sub>6</sub> alcohol<br>Isopropyl-1,1,1,3,3,3-d <sub>6</sub> alcohol |

|                  |                                                  |
|------------------|--------------------------------------------------|
| Formula          | : C <sub>3</sub> D <sub>6</sub> H <sub>2</sub> O |
| Molecular weight | : 66.13 g/mol                                    |
| CAS-No.          | : 3976-29-2                                      |

#### Hazardous components

| Component                                   | Classification                                                 | Concentration |
|---------------------------------------------|----------------------------------------------------------------|---------------|
| <b>2-Propanol-1,1,1,3,3,3-d<sub>6</sub></b> |                                                                |               |
|                                             | Flam. Liq. 2; Eye Irrit. 2A;<br>STOT SE 3; H225, H319,<br>H336 | <= 100 %      |

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

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## 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

No data available

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

Use water spray to cool unopened containers.

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## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

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.

### 6.3 Methods and materials for containment and cleaning up

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).

### 6.4 Reference to other sections

For disposal see section 13.

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## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Use explosion-proof equipment. 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

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Store under inert gas. hygroscopic

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### **Components with workplace control parameters**

| Component                 | CAS-No.   | Value                                                                                                                                                             | Control parameters | Basis                                   |
|---------------------------|-----------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------|-----------------------------------------|
| 2-Propanol-1,1,1,3,3,3-d6 | 3976-29-2 | TWA                                                                                                                                                               | 200.000000 ppm     | USA. ACGIH Threshold Limit Values (TLV) |
|                           | Remarks   | Central Nervous System impairment<br>Upper Respiratory Tract irritation<br>Eye irritation<br>Substances for which there is a Biological Exposure Index or Indices |                    |                                         |

|  |  |                                                                                                                                                                                                                                |                                      |                                                                                         |
|--|--|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------|-----------------------------------------------------------------------------------------|
|  |  | (see BEI® section)<br>Not classifiable as a human carcinogen                                                                                                                                                                   |                                      |                                                                                         |
|  |  | TWA                                                                                                                                                                                                                            | 200 ppm                              | USA. ACGIH Threshold Limit Values (TLV)                                                 |
|  |  | Central Nervous System impairment<br>Upper Respiratory Tract irritation<br>Eye irritation<br>Substances for which there is a Biological Exposure Index or Indices (see BEI® section)<br>Not classifiable as a human carcinogen |                                      |                                                                                         |
|  |  | STEL                                                                                                                                                                                                                           | 400 ppm                              | USA. ACGIH Threshold Limit Values (TLV)                                                 |
|  |  | Central Nervous System impairment<br>Upper Respiratory Tract irritation<br>Eye irritation<br>Substances for which there is a Biological Exposure Index or Indices (see BEI® section)<br>Not classifiable as a human carcinogen |                                      |                                                                                         |
|  |  | STEL                                                                                                                                                                                                                           | 400.000000 ppm                       | USA. ACGIH Threshold Limit Values (TLV)                                                 |
|  |  | Central Nervous System impairment<br>Upper Respiratory Tract irritation<br>Eye irritation<br>Substances for which there is a Biological Exposure Index or Indices (see BEI® section)<br>Not classifiable as a human carcinogen |                                      |                                                                                         |
|  |  | TWA                                                                                                                                                                                                                            | 400.000000 ppm<br>980.000000 mg/m3   | USA. NIOSH Recommended Exposure Limits                                                  |
|  |  | ST                                                                                                                                                                                                                             | 500.000000 ppm<br>1,225.000000 mg/m3 | USA. NIOSH Recommended Exposure Limits                                                  |
|  |  | TWA                                                                                                                                                                                                                            | 400.000000 ppm<br>980.000000 mg/m3   | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants        |
|  |  | The value in mg/m3 is approximate.                                                                                                                                                                                             |                                      |                                                                                         |
|  |  | PEL                                                                                                                                                                                                                            | 400 ppm<br>980 mg/m3                 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
|  |  | STEL                                                                                                                                                                                                                           | 500 ppm<br>1,225 mg/m3               | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |

#### Biological occupational exposure limits

| Component                 | CAS-No.   | Parameters                      | Value        | Biological specimen | Basis                                     |
|---------------------------|-----------|---------------------------------|--------------|---------------------|-------------------------------------------|
| 2-Propanol-1,1,1,3,3,3-d6 | 3976-29-2 | Acetone                         | 40.0000 mg/l | In urine            | ACGIH - Biological Exposure Indices (BEI) |
|                           | Remarks   | End of shift at end of workweek |              |                     |                                           |

## 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

Face shield and safety glasses 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.

### Body Protection

Impervious clothing, 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 respirator with multi-purpose combination (US) or type ABEK (EN 14387) 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.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

|                                                 |                                                                    |
|-------------------------------------------------|--------------------------------------------------------------------|
| a) Appearance                                   | Form: clear, liquid<br>Colour: colourless                          |
| b) Odour                                        | No data available                                                  |
| c) Odour Threshold                              | No data available                                                  |
| d) pH                                           | No data available                                                  |
| e) Melting point/freezing point                 | No data available                                                  |
| f) Initial boiling point and boiling range      | 82 °C (180 °F) - lit.                                              |
| g) Flash point                                  | 16 °C (61 °F) - closed cup                                         |
| h) Evaporation rate                             | No data available                                                  |
| i) Flammability (solid, gas)                    | No data available                                                  |
| j) Upper/lower flammability or explosive limits | No data available                                                  |
| k) Vapour pressure                              | No data available                                                  |
| l) Vapour density                               | No data available                                                  |
| m) Relative density                             | 0.86 g/mL at 25 °C (77 °F) 0.86 g/cm <sup>3</sup> at 25 °C (77 °F) |
| n) Water solubility                             | No data available                                                  |
| 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

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## 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

Vapours may form explosive mixture with air.

### 10.4 Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight.

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

Inhalation: No data available

Dermal: No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

#### Respiratory or skin sensitisation

No data available

#### Germ cell mutagenicity

#### 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.

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

#### Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

#### Specific target organ toxicity - repeated exposure

No data available

#### Aspiration hazard

No data available

#### Additional Information

RTECS: Not available

Central nervous system depression, prolonged or repeated exposure can cause:, Nausea, Headache, Vomiting, narcosis

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

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## 12. ECOLOGICAL INFORMATION

### 12.1 Toxicity

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

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## 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.

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## 14. TRANSPORT INFORMATION

### DOT (US)

UN number: 1219      Class: 3  
Proper shipping name: Isopropanol

Packing group: II

Poison Inhalation Hazard: No

### IMDG

UN number: 1219      Class: 3  
Proper shipping name: ISOPROPANOL

Packing group: II

EMS-No: F-E, S-D

### IATA

UN number: 1219      Class: 3  
Proper shipping name: Isopropanol

Packing group: II

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## 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

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

|                           | CAS-No.   | Revision Date |
|---------------------------|-----------|---------------|
| 2-Propanol-1,1,1,3,3,3-d6 | 3976-29-2 | 1993-04-24    |

### SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

2-Propanol-1,1,1,3,3,3-d6

CAS-No.  
3976-29-2Revision Date  
1993-04-24**Pennsylvania Right To Know Components**

2-Propanol-1,1,1,3,3,3-d6

CAS-No.  
3976-29-2Revision Date  
1993-04-24**New Jersey Right To Know Components**

2-Propanol-1,1,1,3,3,3-d6

CAS-No.  
3976-29-2Revision Date  
1993-04-24**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.

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**16. OTHER INFORMATION****Full text of H-Statements referred to under sections 2 and 3.**

|            |                                                  |
|------------|--------------------------------------------------|
| Eye Irrit. | Eye irritation                                   |
| Flam. Liq. | Flammable liquids                                |
| H225       | Highly flammable liquid and vapour.              |
| H319       | Causes serious eye irritation.                   |
| H336       | May cause drowsiness or dizziness.               |
| STOT SE    | Specific target organ toxicity - single exposure |

**HMIS Rating**

|                        |   |
|------------------------|---|
| Health hazard:         | 2 |
| Chronic Health Hazard: | * |
| Flammability:          | 3 |
| Physical Hazard        | 0 |

**NFPA Rating**

|                    |   |
|--------------------|---|
| Health hazard:     | 2 |
| Fire Hazard:       | 3 |
| Reactivity Hazard: | 0 |

**Further information**

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**Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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