

## SAFETY DATA SHEET

Version 6.6  
Revision Date 09/06/2024  
Print Date 09/07/2024

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

Product name : *tert*-Butanol-d<sub>10</sub>

Product Number : 175889  
Brand : Aldrich  
CAS-No. : 53001-22-2

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

**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, Inhalation (Category 4), H332  
Eye irritation (Category 2A), H319

Specific target organ toxicity - single exposure (Category 3), Respiratory system, Central nervous system, H335, 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 Statements

H225	Highly flammable liquid and vapor.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.
H335	May cause respiratory irritation.
H336	May cause drowsiness or dizziness.

Precautionary Statements

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/ 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.
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

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### SECTION 3: Composition/information on ingredients

#### 3.1 Substances

Synonyms : 2-Methyl-2-propanol-d10

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## tert-Butyl alcohol-d10

Formula : C<sub>4</sub>D<sub>10</sub>O  
Molecular weight : 84.08 g/mol  
CAS-No. : 53001-22-2  
EC-No. : 258-288-0

Component	Classification	Concentration
<b>tert-Butanol-d10</b>		
	Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2A; STOT SE 3; H225, H332, H319, H335, H336	<= 100 %

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

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### 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. 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.

##### 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

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### SECTION 5: Firefighting measures

#### 5.1 Extinguishing media

##### Suitable extinguishing media

Carbon dioxide (CO<sub>2</sub>) Foam 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**

In the event of fire, wear self-contained breathing apparatus.

**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 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.

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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**

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

For precautions see section 2.2.

## 7.2 Conditions for safe storage, including any incompatibilities

### Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

### 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

Component	CAS-No.	Value	Control parameters	Basis
tert-Butanol-d10	53001-22-2	TWA	100 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen		
		TWA	100 ppm 300 mg/m3	USA. NIOSH Recommended Exposure Limits
		ST	150 ppm 450 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	100 ppm 300 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		STEL	150 ppm 450 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		PEL	100 ppm 300 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

### 8.2 Exposure controls

#### Appropriate engineering controls

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

#### Personal protective equipment

##### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

### **Skin protection**

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](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 480 min

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

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](http://www.kcl.de)).

Splash contact

Material: Chloroprene

Minimum layer thickness: 0.65 mm

Break through time: 240 min

Material tested: KCL 720 Camapren®

### **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**

- |                                 |                     |
|---------------------------------|---------------------|
| 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 | No data available   |
| f) Initial boiling point        | 82 °C 180 °F - lit. |

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and boiling range

- |   |   |
|---|---|
| g) Flash point                                  | 11 °C (52 °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) Vapor pressure                               | No data available                               |
| l) Vapor density                                | No data available                               |
| m) Density                                      | 0.893 g/cm <sup>3</sup> 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

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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) .  
Stable

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:

Alkali metals

Alkaline earth metals

Strong acids

Aluminum

Strong oxidizing agents

#### 10.4 Conditions to avoid

Warming.

#### 10.5 Incompatible materials

No data available

#### 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

##### Acute toxicity

LD50 Oral - Rat - male and female - 3,046 mg/kg  
(US-EPA)

Remarks: The value is given in analogy to the following substances: tert-Butanol  
Acute toxicity estimate Inhalation - 4 h - 11.1 mg/l - vapor

(Expert judgment)

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: tert-Butanol

LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg

(US-EPA)

Remarks: The value is given in analogy to the following substances: tert-Butanol

##### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 24 h

(Draize Test)

Remarks: The value is given in analogy to the following substances: tert-Butanol

##### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation.

(US-EPA)

Remarks: The value is given in analogy to the following substances: tert-Butanol

##### Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Remarks: The value is given in analogy to the following substances: tert-Butanol

##### Germ cell mutagenicity

Test Type: In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

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: tert-Butanol

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation



Method: OECD Test Guideline 473

Result: negative

Remarks: The value is given in analogy to the following substances: tert-Butanol  
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: tert-Butanol  
Test Type: sister chromatid exchange assay

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 479

Result: negative

Remarks: The value is given in analogy to the following substances: tert-Butanol  
Test Type: Micronucleus test

Species: Mouse

Cell type: Red blood cells (erythrocytes)

Application Route: Oral

Method: OECD Test Guideline 474

Result: negative

Remarks: The value is given in analogy to the following substances: tert-Butanol

### **Carcinogenicity**

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

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

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

Inhalation - 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: tert-Butanol

Inhalation - May cause drowsiness or dizziness. - Nervous system

Remarks: The value is given in analogy to the following substances: tert-Butanol

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

No data available

#### **Aspiration hazard**

No data available

## **11.2 Additional Information**

drying, cracking of the skin, Skin irritation

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

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## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - > 961 mg/l - 96 h (OECD Test Guideline 203) Remarks: The value is given in analogy to the following substances: tert-Butanol
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 933 mg/l - 48 h (Directive 67/548/EEC, Annex V, C.2.) Remarks: The value is given in analogy to the following substances: tert-Butanol
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - > 976 mg/l - 72 h (OECD Test Guideline 201) Remarks: The value is given in analogy to the following substances: tert-Butanol
Toxicity to bacteria	static test EC50 - Pseudomonas putida - > 10,000 mg/l - 16 h (DIN 38 412 Part 8) Remarks: The value is given in analogy to the following substances: tert-Butanol  static test EC10 - Pseudomonas putida - 6,900 mg/l - 16 h (DIN 38 412 Part 8) Remarks: The value is given in analogy to the following substances: tert-Butanol
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	semi-static test EC50 - Daphnia magna (Water flea) - > 100 mg/l - 21 d (OECD Test Guideline 211) Remarks: The value is given in analogy to the following substances: tert-Butanol  semi-static test NOEC - Daphnia magna (Water flea) - 100 mg/l - 21 d (OECD Test Guideline 211) Remarks: The value is given in analogy to the following substances: tert-Butanol

## 12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 56 d  
Result: 66 % - Inherently biodegradable.  
Remarks: (ECHA)  
The value is given in analogy to the following substances: tert-Butanol

## 12.3 Bioaccumulative potential

No data available

## 12.4 Mobility in soil

No data available

## 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

## 12.6 Endocrine disrupting properties

No data available

## 12.7 Other adverse effects

No data available

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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.

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## SECTION 14: Transport information

### DOT (US)

UN number: 1120 Class: 3 Packing group: II  
Proper shipping name: Butanols  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

UN number: 1120 Class: 3 Packing group: II EMS-No: F-E, S-D  
Proper shipping name: BUTANOLS

### IATA

UN number: 1120 Class: 3 Packing group: II  
Proper shipping name: Butanols

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## SECTION 15: Regulatory information

### CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

### SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

### SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

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

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

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

tert-Butanol-d10	53001-22-2	>= 90 - <= 100 %
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### US State Regulations

#### Massachusetts Right To Know

tert-Butanol-d10	53001-22-2
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#### Pennsylvania Right To Know

tert-Butanol-d10	53001-22-2
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#### Maine Chemicals of High Concern

Product does not contain any listed chemicals

#### Vermont Chemicals of High Concern

Product does not contain any listed chemicals

#### Washington Chemicals of High Concern

Product does not contain any listed chemicals

### The ingredients of this product are reported in the following inventories:

**TSCA** : Product contains substance(s) not listed on TSCA inventory.

### TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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## SECTION 16: Other information

### 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 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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Details in analogy to the undeuterated compound.

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