

## SAFETY DATA SHEET

Version 6.9  
Revision Date 10/15/2024  
Print Date 10/16/2024

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

Product name : (±)-1,3-Butanediol

Product Number : B84785  
Brand : Sigma-Aldrich  
CAS-No. : 107-88-0

**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**

Not a hazardous substance or mixture.

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

No hazard pictogram, no signal word, no hazard statement(s), no precautionary statement(s) required.

## 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 : 1,3-Butylene glycol

Formula :  $C_4H_{10}O_2$   
Molecular weight : 90.12 g/mol  
CAS-No. : 107-88-0  
EC-No. : 203-529-7

No components need to be disclosed according to the applicable regulations.

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### SECTION 4: First aid measures

#### 4.1 Description of first-aid measures

##### If inhaled

After inhalation: fresh air.

##### 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. Remove contact lenses.

##### If swallowed

After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

#### 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.

Vapors are heavier than air and may spread along floors.  
Forms explosive mixtures with air on intense heating.  
Development of hazardous combustion gases or vapours possible in the event of fire.

### **5.3 Advice for firefighters**

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

### **5.4 Further information**

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. 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.

### **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. 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**

For precautions see section 2.2.

### **7.2 Conditions for safe storage, including any incompatibilities**

#### **Storage conditions**

Tightly closed.

hygroscopic

#### **Storage class**

Storage class (TRGS 510): 10: Combustible liquids

### **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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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Change contaminated clothing. 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: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

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: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

##### Respiratory protection

Not required; except in case of aerosol formation.

##### Control of environmental exposure

Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |               |   |
|---------------|---|
| a) Appearance | Form: liquid<br>Color: colorless, clear |
| b) Odor       | odorless                                |

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c) Odor Threshold	No data available
d) pH	6.0 - 7.0 at 20 °C (68 °F)
e) Melting point/freezing point	Melting point/freezing point: -57 °C (-71 °F) - ISO 3016
f) Initial boiling point and boiling range	203 - 204 °C 397 - 399 °F - lit.
g) Flash point	108 °C (226 °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: 12.6 %(V) Lower explosion limit: 1.9 %(V)
k) Vapor pressure	0.08 hPa at 20 °C (68 °F)
l) Vapor density	3.11 - (Air = 1.0)
m) Density	1.005 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	500 g/l at 20 °C (68 °F) - OECD Test Guideline 105 - miscible
o) Partition coefficient: n-octanol/water	log Pow: -0.9 at 25 °C (77 °F) - Bioaccumulation is not expected.
p) Autoignition temperature	410 °C (770 °F) at 1,019 hPa - DIN 51794
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

Surface tension	72.6 mN/m at 1g/l at 20 °C (68 °F) - OECD Test Guideline 115
Dissociation constant	15.5 at 25 °C (77 °F) - OECD Test Guideline 112
Relative vapor density	3.11 - (Air = 1.0)

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.  
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

## 10.2 Chemical stability

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

## 10.3 Possibility of hazardous reactions

Violent reactions possible with:

Oxidizing agents

Acid anhydrides

acid halides

## 10.4 Conditions to avoid

Avoid moisture.

Strong heating.

## 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 - 22,800 mg/kg

Remarks: (ECHA)

Inhalation: No data available

LD50 Dermal - Rabbit - > 20,000 mg/kg

Remarks: (RTECS)

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: Mild skin irritation - 24 h

Remarks: (RTECS)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

Remarks: (External MSDS)

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Species: Rat

Cell type: Bone marrow

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Application Route: Oral

Result: negative  
Remarks: (ECHA)

Test Type: in vivo assay  
Species: Rat

Application Route: Oral

Result: negative  
Remarks: (ECHA)

### **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**

No data available

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

No data available

### **Aspiration hazard**

No data available

## **11.2 Additional Information**

Repeated dose toxicity - No data available

RTECS: EK0440000

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

Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.

Handle in accordance with good industrial hygiene and safety practice.

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## **SECTION 12: Ecological information**

### **12.1 Toxicity**

Toxicity to fish	semi-static test LC50 - <i>Oryzias latipes</i> (Orange-red killifish) - > 100 mg/l - 96 h (OECD Test Guideline 203)
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Remarks: The value is given in analogy to the following substances:  
butane-1,4-diol

Toxicity to daphnia and other aquatic invertebrates	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: butane-1,4-diol
Toxicity to algae	static test ErC50 - Desmodesmus subspicatus (green algae) - > 1,070 mg/l - 72 h (OECD Test Guideline 201)  static test NOEC - Desmodesmus subspicatus (green algae) - > 1,070 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC50 - activated sludge - > 100 mg/l - 3 h (OECD Test Guideline 209)

## **12.2 Persistence and degradability**

Biodegradability      aerobic - Exposure time 29 d  
Result: 81 % - Readily biodegradable.  
(OECD Test Guideline 301B)

## **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)

Not dangerous goods

### IMDG

Not dangerous goods

### IATA

Not dangerous goods

### Further information

Not classified as dangerous in the meaning of transport regulations.

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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** : No SARA Hazards

**SARA 313** : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

### Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

The following chemical(s) are listed under the U.S. Clean Air Act Section 111 SOCM I Intermediate or Final VOC's (40 CFR 60.489):

butane-1,3-diol	107-88-0	>= 90 - <= 100 %
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### Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

### **US State Regulations**

#### **Massachusetts Right To Know**

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

#### **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 : All substances listed as active on the 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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