

# SAFETY DATA SHEET

Version 6.4  
Revision Date 11/25/2023  
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## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : 1,3-Propanedisulfonic acid

Product Number : P8454

Brand : Aldrich

CAS-No. : 21668-77-9

### 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

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## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

#### GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Skin corrosion (Category 1B), H314

Serious eye damage (Category 1), H318

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	
H314	Causes severe skin burns and eye damage.
Precautionary Statements	
P264	Wash skin thoroughly after handling.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P330 + P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P363	Wash contaminated clothing before reuse.
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

### SECTION 3: Composition/information on ingredients

#### 3.2 Mixtures

Formula	:	C <sub>3</sub> H <sub>8</sub> O <sub>6</sub> S <sub>2</sub>
Molecular weight	:	204.22 g/mol

Component	Classification	Concentration
<b>1,3-propanedisulfonic acid</b>		
CAS-No.	21668-77-9	Skin Corr. 1B; Eye Dam. 1; H314, H318
EC-No.	679-154-1	>= 70 - < 90 %
<b>n-butanol</b>		
CAS-No.	71-36-3	Flam. Liq. 3; Acute Tox. 4;
EC-No.	200-751-6	Skin Irrit. 2; Eye Dam. 1;
Index-No.	603-004-00-6	STOT SE 3; H226, H302,
Registration number	01-2119484630-38-XXXX	H315, H318, H335, H336 Concentration limits: >= 20 %: STOT SE 3, H335; >= 20 %: STOT SE 3, H336;

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**

First aiders need to protect themselves. 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. Call a physician immediately.

#### **In case of eye contact**

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

#### **If swallowed**

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

### 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**

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

Sulfur oxides

Mixture with combustible ingredients.

Development of hazardous combustion gases or vapours possible in the event of fire.

### 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

Suppress (knock down) gases/vapors/mists with a water spray jet. 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. 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. Keep locked up or in an area accessible only to qualified or authorized persons.

#### Storage class

Storage class (TRGS 510): 8A: Combustible, corrosive hazardous materials

### 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

Component	CAS-No.	Value	Control parameters	Basis
n-butanol	71-36-3	TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
		C	50 ppm 150 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
Remarks			Potential for dermal absorption	

		TWA	100 ppm 300 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants	
		C	50 ppm 150 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)	
		Skin			

## 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). Tightly fitting safety goggles

#### Skin protection

required

#### Body Protection

protective clothing

#### Respiratory protection

Recommended Filter type: Filter type ABEK

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.

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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 No data available

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	and boiling range
g)	Flash point (No data available)
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 No data available 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 Not classified as explosive.
t)	Oxidizing properties none

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 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

no information available

### 10.5 Incompatible materials

Strong oxidizing agents

### 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**

Oral: No data available

Inhalation: No data available

Acute toxicity estimate Dermal - > 5,000 mg/kg  
(Calculation method)

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

Remarks: Mixture causes burns.

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

Remarks: Mixture causes serious eye damage.

Risk of blindness!

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

No data available

##### **Germ cell mutagenicity**

No data available

##### **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**

corrosive effects, Redness, 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.

## **Components**

### **1,3-propanedisulfonic acid**

#### **Acute toxicity**

Oral: No data available  
Inhalation: No data available  
Dermal: No data available

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

Remarks: No data available

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

Remarks: No data available

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

No data available

#### **Germ cell mutagenicity**

No data available

#### **Carcinogenicity**

No data available

#### **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

## **n-butanol**

#### **Acute toxicity**

LD50 Oral - Rat - 790 mg/kg  
Remarks: Liver:Fatty liver degeneration.  
Kidney, Ureter, Bladder:Other changes.  
Blood:Other changes.  
(RTECS)  
Inhalation: No data available  
LD50 Dermal - Rabbit - male - 3,430 mg/kg  
(OECD Test Guideline 402)

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

Skin - Rabbit  
Result: Skin irritation - 2 h  
Remarks: (ECHA)  
Remarks: (Regulation (EC) No 1272/2008, Annex VI)

**Serious eye damage/eye irritation**

Eyes - Rabbit

Result: Irreversible effects on the eye

(OECD Test Guideline 405)

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

**Respiratory or skin sensitization**

No data available

**Germ cell mutagenicity**

Test Type: Mutagenicity (mammal cell test): micronucleus.

Test system: Chinese hamster lung cells

Result: negative

Remarks: (ECHA)

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster lung cells

Result: negative

Method: OECD Test Guideline 474

Species: Mouse - male and female

Result: negative

**Carcinogenicity**

No data available

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

May cause respiratory irritation. - Respiratory Tract, Skin, Eyes

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

May cause drowsiness or dizziness.

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

**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 Endocrine disrupting properties

No data available

## 12.7 Other adverse effects

No data available

### Components

#### 1,3-propanedisulfonic acid

No data available

### n-butanol

Toxicity to fish	static test LC50 - Pimephales promelas (fathead minnow) - 1,376 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 1,328 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 225 mg/l - 96 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC50 - Pseudomonas putida - 4,390 mg/l - 17 h (DIN 38421 TEIL 8)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	semi-static test EC50 - Daphnia magna (Water flea) - 18 mg/l - 21 d (OECD Test Guideline 211)

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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: 1760 Class: 8 Packing group: II  
Proper shipping name: Corrosive liquids, n.o.s. (1,3-propanedisulfonic acid)  
Reportable Quantity (RQ): 100 lbs  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

UN number: 1760 Class: 8 Packing group: II EMS-No: F-A, S-B  
Proper shipping name: CORROSIVE LIQUID, N.O.S. (1,3-propanedisulfonic acid)

### IATA

UN number: 1760 Class: 8 Packing group: II  
Proper shipping name: Corrosive liquid, n.o.s. (1,3-propanedisulfonic acid)

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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

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.

### SARA 311/312 Hazards

Acute Health Hazard, Chronic Health Hazard

:

**Reportable Quantity** F003 lbs

### Massachusetts Right To Know Components

	CAS-No.	Revision Date
water	7732-18-5	
n-butanol	71-36-3	2020-07-14

### Pennsylvania Right To Know Components

n-butanol	CAS-No. 71-36-3	Revision Date 2020-07-14
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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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