

SAFETY DATA SHEET

Version 8.6
Revision Date 07/01/2021
Print Date 10/28/2021**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 2-Butyne-1,4-diol (not stabilised) for synthesis

Product Number : 8.01537
Catalogue No. : 801537
Brand : Millipore
Index-No. : 603-076-00-9
CAS-No. : 110-65-6**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Identified uses : Chemical for synthesis

1.3 Details of the supplier of the safety data sheetCompany : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATESTelephone : +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)**Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Skin corrosion (Category 1B), H314
Serious eye damage (Category 1), H318
Skin sensitization (Category 1), H317
Specific target organ toxicity - repeated exposure (Category 2), H373

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)

H301 + H311 + H331

H314

H317

H373

Toxic if swallowed, in contact with skin or if inhaled.

Causes severe skin burns and eye damage.

May cause an allergic skin reaction.

May cause damage to organs through prolonged or repeated exposure.

Precautionary statement(s)

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.

P272

Contaminated work clothing must not be allowed out of the workplace.

P280

Wear protective gloves/ protective clothing/ eye protection/ face protection.

P301 + P310 + P330

IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.

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.

P314

Get medical advice/ attention if you feel unwell.

P333 + P313

If skin irritation or rash occurs: Get medical advice/ attention.

P362

Take off contaminated clothing and wash before reuse.

P403 + P233

Store in a well-ventilated place. Keep container tightly closed.

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

3.1 Substances

Formula : C₄H₆O₂
Molecular weight : 86.09 g/mol
CAS-No. : 110-65-6
EC-No. : 203-788-6
Index-No. : 603-076-00-9

Component	Classification	Concentration
but-2-yne-1,4-diol	Acute Tox. 3; Skin Corr. 1B; Eye Dam. 1; Skin	<= 100 %

	Sens. 1; STOT RE 2; H301, H331, H311, H314, H318, H317, H373 Concentration limits: >= 50 %: Skin Corr. 1B, H314; 25 - < 50 %: Skin Irrit. 2, H315; 25 - < 50 %: Eye Irrit. 2, H319;	
--	--	--

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. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible. 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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water Foam Carbon dioxide (CO₂) 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

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

none

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid generation and inhalation of dusts in all circumstances. 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

No special precautionary measures necessary.

6.3 Methods and materials for containment and cleaning up

Observe possible material restrictions (see sections 7 and 10). Take up carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture.

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

Protected from light. Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Recommended storage temperature see product label.

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

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

Contains no substances with occupational exposure limit values.

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

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: 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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: 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

Body Protection

protective clothing

Respiratory protection

required when dusts 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

No special precautionary measures necessary.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: solid Color: light yellow
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: 56 - 58 °C (133 - 136 °F)
f) Initial boiling point and boiling range	238 °C 460 °F at 1,013 hPa
g) Flash point	152 °C (306 °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	< 0.1 hPa at 55 °C (131 °F)
l) Vapor density	No data available
m) Relative density	No data available
n) Water solubility	3,740 g/l at 20 °C (68 °F)
o) Partition coefficient: n-octanol/water	log Pow: -0.73 at 25 °C (77 °F)
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

Bulk density	500 kg/m ³
--------------	-----------------------

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.

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

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

Air Avoid moisture.

Strong heating.

10.5 Incompatible materials

Strong oxidizing agents, Strong bases, Strong acids, Mercury/mercury oxides., Halides

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male - 132 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - 0.669 mg/l

(OECD Test Guideline 403)

LD50 Dermal - 400 mg/kg

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Causes burns.

(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Risk of serious damage to eyes.

(OECD Test Guideline 405)

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Test Type: Chromosome aberration test in vitro

Test system: fibroblast

Metabolic activation: with and without metabolic activation

Result: negative

Test Type: Micronucleus test

Species: Mouse

Application Route: Intraperitoneal

Method: Mutagenicity (micronucleus test)

Result: negative

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
No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

May cause damage to organs through prolonged or repeated exposure. **Aspiration hazard**
No data available

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - NOAEL (No observed adverse effect level) - 1 mg/kg - LOAEL (Lowest observed adverse effect level) - 10 mg/kg

prolonged or repeated exposure can cause:, narcosis, Central nervous system depression,
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to algae static test EC50 - Desmodesmus subspicatus (green algae) - 1,048 mg/l - 72 h (OECD Test Guideline 201)

12.2 Persistence and degradability

Biodegradability Result: - Readily biodegradable.
Remarks: 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

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 for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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

UN number: 2716 Class: 6.1 Packing group: III
Proper shipping name: 1,4-Butynediol
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 2716 Class: 6.1 Packing group: III EMS-No: F-A, S-A
Proper shipping name: 1,4-BUTYNEDIOL

IATA

UN number: 2716 Class: 6.1 Packing group: III
Proper shipping name: 1,4-Butynediol

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.

Massachusetts Right To Know Components

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

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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

Version: 8.6

Revision Date: 07/01/2021

Print Date: 10/28/2021