Chemical Safety Data Sheet MSDS / SDS

But-2-yne-1,4-diol SDS

Revision Date:2024-04-25 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking

Product identifier

Product name: But-2-yne-1,4-diol

CAS: 110-65-6

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

Relevant identified uses: For R&D use only. Not for medicinal, household or other use.

Uses advised against: none

Company Identification

Company: Chemicalbook.in

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

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SECTION 2: Hazards identification

Classification of the substance or mixture

Acute toxicity - Category 3, Oral
Acute toxicity - Category 4, Dermal

Skin corrosion, Sub-category 1B
Skin sensitization, Category 1
Acute toxicity - Category 3, Inhalation
Specific target organ toxicity – repeated exposure, Category 2

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H301 Toxic if swallowed
H312 Harmful in contact with skin
H314 Causes severe skin burns and eye damage
H317 May cause an allergic skin reaction
H331 Toxic if inhaled
H373 May cause damage to organs through prolonged or repeated exposure

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P272 Contaminated work clothing should not be allowed out of the workplace.
P271 Use only outdoors or in a well-ventilated area.

Response

P301+P316 IF SWALLOWED: Get emergency medical help immediately.
P321 Specific treatment (see ... on this label).
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P317 Get medical help.
P362+P364 Take off contaminated clothing and wash it before reuse.
P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P363 Wash contaminated clothing before reuse.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P316 Get emergency medical help immediately.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P333+P317 If skin irritation or rash occurs: Get medical help.
P319 Get medical help if you feel unwell.

Storage

P405 Store locked up.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	But-2-yne-1,4-diol
Common names and synonyms:	But-2-yne-1,4-diol
CAS number:	110-65-6
EC number:	203-788-6
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Half-upright position. Refer immediately for medical attention.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer immediately for medical attention.

Following eye contact

Rinse with plenty of water (remove contact lenses if easily possible). Refer immediately for medical attention.

Following ingestion

Rinse mouth. Do NOT induce vomiting. Refer immediately for medical attention.

Most important symptoms/effects, acute and delayed

May cause dermatitis. (USCG, 1999)

Indication of immediate medical attention and special treatment needed, if necessary

Basic Treatment: Establish a patent airway (oropharyngeal or nasopharyngeal airway, if needed). Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for shock and treat if necessary . Monitor for pulmonary edema and treat if necessary . Anticipate seizures and treat if necessary . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with 0.9% saline (NS) during transport . Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool. Administer activated charcoal . Higher alcohols (>3 carbons) and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

If material on fire or involved in fire: Do not extinguish fire unless flow can be stopped. Use water in flooding quantities as fog. Solid streams fo water may be ineffective Cool all affected containers with flooding quantities of water. Use "alcohol" foam, dry chemical or carbon dioxide. Keep run-off water out of sewers and water sources.

Specific hazards arising from the chemical

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]: Combustible material: may burn but does not ignite readily. When heated, vapors may form explosive mixtures with air: indoors, outdoors and sewers explosion hazards. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Contact with metals may evolve flammable hydrogen gas. Containers may explode when heated. Runoff may pollute waterways. Substance may be transported in a

molten form. (ERG, 2016)

Special protective actions for fire-fighters

Use water spray, alcohol-resistant foam, dry powder, carbon dioxide.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Evacuate danger area! Consult an expert! Personal protection: chemical protection suit including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

Environmental precautions

Evacuate danger area! Consult an expert! Personal protection: chemical protection suit including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Separated from incompatible materials. See Chemical Dangers. Cool. Store in an area without drain or sewer access.The storage temperature should be kept below 40 deg C and storage times longer than a few months should be avoided because the butynediol flakes tend to set up.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

MAK: 0.36 mg/m3, 0.1 ppm; peak limitation category: I(1); skin absorption (H); sensitization of skin (SH); pregnancy risk group: C.EU-OEL: 0.5 mg/m3 as TWA

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear face shield or eye protection in combination with breathing protection if powder.

Skin protection

Protective clothing. Protective gloves.

Respiratory protection

Use ventilation (not if powder).

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	1,4-butynediol is a white to light-brown solid or brownish-yellow aqueous solution. Solid sinks and mixes with water. (USCG, 1999)
Colour:	Plates from benzene and ethyl acetate

Odour:	no data available
Melting point/freezing point:	8°C(lit.)
Boiling point or initial boiling point and boiling range:	238°C(lit.)
Flammability:	Combustible.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	120°C(lit.)
Auto-ignition temperature:	335°C
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	Insoluble in benzene; slightly soluble in ethyl ether, choroform; very soluble in ethanol, acetone, methanol
Partition coefficient n-octanol/water:	log Kow = -0.93 (est)
Vapour pressure:	<0.1 mm Hg (55 °C)
Density and/or relative density:	1.2
Relative vapour density:	(air = 1): 3.0
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Decomposes on heating. This produces toxic and corrosive fumes. Reacts violently with anhydrides, acid chlorides, mercury salts and alkaline hydroxides or chlorides. This generates explosion hazard.

Chemical stability

no data available

Possibility of hazardous reactions

Pure BUTYNEDIOL is non-explosive. Small amounts of certain impurities-alkali hydroxides, alkaline earth hydroxides, halides-may cause explosive decomposition upon distillation. Butynediol should not be treated with basic catalysts in the absence of a solvent at room temperature, and its stability is less with elevated temperatures. In strong acids, contamination with mercury salts can also result in violent decomposition. [NFPA 491M 1991].

Conditions to avoid

no data available

Incompatible materials

The pure diol may be distilled unchanged, but traces of alkali or alkaline earth hydroxides or halides may cause explosive decomposition during distillation. In presence of strong acids, mercury salts may cause violent decomposition of the diol.

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and fumes and may explode.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Guniea pig oral 130 mg/kg

Inhalation: no data available

Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

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

STOT-single exposure

Corrosive. Inhalation may cause lung oedema, but only after initial corrosive effects on eyes and/or airways have become manifest. Medical observation is indicated.

STOT-repeated exposure

The substance may have effects on the blood. This may result in anaemia. The substance may have effects on the kidneys and liver. This may result in tissue lesions. Repeated or prolonged contact may cause skin sensitization.

Aspiration hazard

A harmful contamination of the air will not or will only very slowly be reached on evaporation of this substance at 20°C; on spraying or dispersing, however, much faster.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 Pimephales promelas (Fathead minnow) 53.6 mg/L/96 hr (confidence limit 49.3-58.3 mg/L), flow-through bioassay with measured concentrations, 25.1 deg C, dissolved oxygen 6.8 mg/L, hardness 46.5 mg/L calcium carbonate, alkalinity 43.5 mg/L calcium carbonate, and pH 7.7

Toxicity to daphnia and other aquatic invertebrates: EC50 Daphnia magna 26.8 mg/L48 hr (nominal concentration) immobilization, static test. NOTE: At 100 mg/L all daphnids were immobile after 48 hours.

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: Biodegradation of 1,4-butynediol was 90% complete in 4 days using an initial concentration of 500 mg/L and a sewage sludge inoculum concentration of 500 mg/L(1).

Bioaccumulative potential

An estimated BCF of 0.12 was calculated in fish for 1,4-butynediol(SRC), using a water solubility of 3.74X10+6 mg/L(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

The Koc of 1,4-butynediol is estimated as 1(SRC), using a water solubility of 3.74X10+6 mg/L(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that 1,4-butynediol is expected to have very high mobility in soil.

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN2716 (For reference only, please check.)
IMDG: UN2716 (For reference only, please check.)
IATA: UN2716 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: 1,4-BUTYNEDIOL (For reference only, please check.)
IMDG: 1,4-BUTYNEDIOL (For reference only, please check.)
IATA: 1,4-BUTYNEDIOL (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)
IMDG: 6.1 (For reference only, please check.)
IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: III (For reference only, please check.)
IMDG: III (For reference only, please check.)
IATA: III (For reference only, please check.)

Environmental hazards

ADR/RID: No
IMDG: No
IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home

HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm

IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple

ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg

Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp

ECHA - European Chemicals Agency, website: https://echa.europa.eu/

Other Information

There is no odour warning even when toxic concentrations are present. Insufficient data are available on the effect of this substance on human health, therefore utmost care must be taken.