



# SAFETY DATA SHEETS

According to the UN GHS revision 9

Version: 1.0  
Creation Date: July 15, 2019  
Revision Date: July 15, 2019

## SECTION 1: Identification

### 1.1 GHS Product identifier

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

### 1.2 Other means of identification

**Product number** -

**Other names** 2-Butyne-1,4-diol; 1,4-Dihydroxy-2-butyne; 1,2-Dihydroxydimethylacetylene

### 1.3 Recommended use of the chemical and restrictions on use

**Identified uses** Industrial and scientific research use.

**Uses advised against** no data available

### 1.4 Supplier's details

**Company** Shanghai Yien Chemical Technology Co., Ltd  
**Address** Building 6, 28 Yingong Road, Fengxian District, Shanghai  
Chemical Industry Zone, Shanghai, 201400, China  
**Telephone** +86-400-133-2688

### 1.5 Emergency phone number

**Emergency phone number** +86-400-133-2688

**Service hours** Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

## SECTION 2: Hazard identification

### 2.1 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

### 2.2 GHS label elements, including precautionary statements

**Pictogram(s)**



**Signal word**

Danger

|                                   |   |
|-----------------------------------|---|
| <b>Hazard statement(s)</b>        | H301 Toxic if swallowed<br>H312 Harmful in contact with skin<br>H314 Causes severe skin burns and eye damage<br>H317 May cause an allergic skin reaction<br>H331 Toxic if inhaled<br>H373 May cause damage to organs through prolonged or repeated exposure   |
| <b>Precautionary statement(s)</b> |   |
| <b>Prevention</b>                 | P264 Wash ... thoroughly after handling.<br>P270 Do not eat, drink or smoke when using this product.<br>P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...<br>P260 Do not breathe dust/fume/gas/mist/vapours/spray.<br>P261 Avoid breathing dust/fume/gas/mist/vapours/spray.<br>P272 Contaminated work clothing should not be allowed out of the workplace.<br>P271 Use only outdoors or in a well-ventilated area.   |
| <b>Response</b>                   | P301+P316 IF SWALLOWED: Get emergency medical help immediately.<br>P321 Specific treatment (see ... on this label).<br>P330 Rinse mouth.<br>P302+P352 IF ON SKIN: Wash with plenty of water/...<br>P317 Get medical help.<br>P362+P364 Take off contaminated clothing and wash it before reuse.<br>P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.<br>P363 Wash contaminated clothing before reuse.<br>P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.<br>P316 Get emergency medical help immediately.<br>P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.<br>P333+P317 If skin irritation or rash occurs: Get medical help.<br>P319 Get medical help if you feel unwell. |
| <b>Storage</b>                    | P405 Store locked up.<br>P403+P233 Store in a well-ventilated place. Keep container tightly closed.   |
| <b>Disposal</b>                   | 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.   |

### 2.3 Other hazards which do not result in classification

no data available

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

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

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## SECTION 4: First-aid measures

### 4.1 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.

### **4.2 Most important symptoms/effects, acute and delayed**

May cause dermatitis. (USCG, 1999)

### **4.3 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

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## **SECTION 5: Fire-fighting measures**

### **5.1 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 of 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.

### **5.2 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)

### **5.3 Special protective actions for fire-fighters**

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

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## **SECTION 6: Accidental release measures**

### **6.1 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.

### **6.2 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.

### **6.3 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.

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## SECTION 7: Handling and storage

### 7.1 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.

### 7.2 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.

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Occupational Exposure limit values

MAK: 0.36 mg/m<sup>3</sup>, 0.1 ppm; peak limitation category: I(1); skin absorption (H); sensitization of skin (SH); pregnancy risk group: C. EU-OEL: 0.5 mg/m<sup>3</sup> as TWA

#### Biological limit values

no data available

### 8.2 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.

### 8.3 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

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## SECTION 9: Physical and chemical properties and safety characteristics

|   |  |
|---|--|
| <b>Physical state</b>   | 1,4-butynediol is a white to light-brown solid or brownish-yellow aqueous solution. Solid sinks and mixes with water. (USCG, 1999) |
| <b>Colour</b>   | Plates from benzene and ethyl acetate  |
| <b>Odour</b>  | no data available  |
| <b>Melting point/freezing point</b>                             | 8°C(lit.)  |
| <b>Boiling point or initial boiling point and boiling range</b> | 238°C(lit.)  |
| <b>Flammability</b>   | Combustible.   |

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

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## SECTION 10: Stability and reactivity

### 10.1 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.

### 10.2 Chemical stability

no data available

### 10.3 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].

### 10.4 Conditions to avoid

no data available

### 10.5 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.

### 10.6 Hazardous decomposition products

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

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## SECTION 11: Toxicological information

### Acute toxicity

- Oral: LD50 Guinea 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.

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## SECTION 12: Ecological information

### 12.1 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/L/48 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

### 12.2 Persistence and degradability

AEROBIC: Biodegradation of 1,4-butyndiol 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).

### 12.3 Bioaccumulative potential

An estimated BCF of 0.12 was calculated in fish for 1,4-butyndiol(SRC), using a water solubility of  $3.74 \times 10^{-6}$  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).

### 12.4 Mobility in soil

The Koc of 1,4-butyndiol is estimated as 1(SRC), using a water solubility of  $3.74 \times 10^{-6}$  mg/L(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that 1,4-butyndiol is expected to have very high mobility in soil.

### 12.5 Other adverse effects

no data available

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## SECTION 13: Disposal considerations

## 13.1 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.

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## SECTION 14: Transport information

### 14.1 UN Number

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

IMDG: UN2716 (For reference only, please check.)

IATA: UN2716 (For reference only, please check.)

### 14.2 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.)

### 14.3 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.)

### 14.4 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.)

### 14.5 Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

### 14.6 Special precautions for user

no data available

### 14.7 Transport in bulk according to IMO instruments

no data available

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## SECTION 15: Regulatory information

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

| Chemical name  | Common names and synonyms | CAS number | EC number |
|--|---------------------------|------------|-----------|
| But-2-yne-1,4-diol   | But-2-yne-1,4-diol        | 110-65-6   | 203-788-6 |
| 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.   |
| Philippines Inventory of Chemicals and Chemical Substances (PICCS)     |                           |            | Listed.   |
| Vietnam National Chemical Inventory                                    |                           |            | Listed.   |
| Chinese Chemical Inventory of Existing Chemical Substances             |                           |            | Listed.   |

|                                      |         |
|--------------------------------------|---------|
| (China IECSC)                        |         |
| Korea Existing Chemicals List (KECL) | Listed. |

## SECTION 16: Other information

### Information on revision

**Creation Date**                      July 15, 2019  
**Revision Date**                      July 15, 2019

### 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](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.

**Any questions regarding this SDS, Please send your inquiry to [sds@xixisys.com](mailto:sds@xixisys.com)**

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