

## Material Safety Data Sheet

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Version 2.2  
Regulation (EC) No 1907/2006

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1 - Product and Company Information

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Product Name 2-BUTYNE-1,4-DIOL, CRYSTALLIZED  
Product Number 19180  
  
Company Sigma-Aldrich Company Ltd.  
The Old Brickyard  
New Road, Gillingham SP8 4XT  
United Kingdom  
  
Technical Phone # 44-(0)-1747-833000  
Fax 44-(0)-1747-833313  
E-mail Address eurtechserv@sial.com  
Emergency Phone # 44-(0)-1747-833100

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2 - Hazards Identification

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SPECIAL INDICATION OF HAZARDS TO HUMANS AND THE ENVIRONMENT  
Harmful in contact with skin. Toxic by inhalation and if  
swallowed. Causes burns. May cause sensitization by skin contact.  
Harmful: danger of serious damage to health by prolonged exposure  
if swallowed.

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3 - Composition/Information on Ingredients

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Product Name	CAS #	EC no	Annex I Index Number
2-BUTYNE-1,4-DIOL	110-65-6	203-788-6	603-076-00-9
Formula	C4H6O2		
Molecular Weight	86.09 AMU		
Synonyms	Agrisynth B3D * Bis(hydroxymethyl)acetylene * 2-Butin-1,4-diol (Czech) * Butynediol		

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4 - First Aid Measures

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## AFTER INHALATION

If inhaled, remove to fresh air. If not breathing give  
artificial respiration. If breathing is difficult, give oxygen.

## AFTER SKIN CONTACT

In case of skin contact, flush with copious amounts of water for  
at least 15 minutes. Remove contaminated clothing and shoes.  
Call a physician.

## AFTER EYE CONTACT

In case of contact with eyes, flush with copious amounts of  
water for at least 15 minutes. Assure adequate flushing by  
separating the eyelids with fingers. Call a physician.

## AFTER INGESTION

If swallowed, wash out mouth with water provided person is  
conscious. Call a physician immediately.

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## 5 - Fire Fighting Measures

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### EXTINGUISHING MEDIA

Suitable: Carbon dioxide, dry chemical powder, or appropriate foam.

### SPECIAL RISKS

Specific Hazard(s): Emits toxic fumes under fire conditions.  
Explosion Hazards: Container explosion may occur under fire conditions.

### SPECIAL PROTECTIVE EQUIPMENT FOR FIREFIGHTERS

Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.

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## 6 - Accidental Release Measures

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PERSONAL PRECAUTION PROCEDURES TO BE FOLLOWED IN CASE OF LEAK OR SPILL  
Evacuate area.

### PROCEDURE(S) OF PERSONAL PRECAUTION(S)

Wear self-contained breathing apparatus, rubber boots, and heavy rubber gloves.

### METHODS FOR CLEANING UP

Sweep up, place in a bag and hold for waste disposal. Avoid raising dust. Ventilate area and wash spill site after material pickup is complete.

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## 7 - Handling and Storage

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### HANDLING

Directions for Safe Handling: Do not breathe dust. Do not get in eyes, on skin, on clothing. Avoid prolonged or repeated exposure.

### STORAGE

Conditions of Storage: Keep tightly closed.

SPECIAL REQUIREMENTS: Air and moisture sensitive. Handle and store under inert gas.

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## 8 - Exposure Controls / Personal Protection

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### ENGINEERING CONTROLS

Use only in a chemical fume hood. Safety shower and eye bath.

### GENERAL HYGIENE MEASURES

Wash contaminated clothing before reuse. Discard contaminated shoes. Wash thoroughly after handling.

### PERSONAL PROTECTIVE EQUIPMENT

Respiratory Protection: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator.  
Hand Protection: Compatible chemical-resistant gloves.  
Eye Protection: Chemical safety goggles.

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## 9 - Physical and Chemical Properties

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Appearance	Physical State: Solid. Color: Beige	
Property	Value	At Temperature or Pressure
pH	N/A	
BP/BP Range	238 °C	760 mmHg
MP/MP Range	54 °C	
Flash Point	152 °C	Method: closed cup
Flammability	N/A	
Autoignition Temp	N/A	
Oxidizing Properties	N/A	
Explosive Properties	N/A	
Explosion Limits	N/A	
Vapor Pressure	< 0.1 mmHg	20 °C
SG/Density	N/A	
Partition Coefficient	N/A	
Viscosity	N/A	
Vapor Density	N/A	
Saturated Vapor Conc.	N/A	
Evaporation Rate	N/A	
Bulk Density	N/A	
Decomposition Temp.	N/A	
Solvent Content	N/A	
Water Content	N/A	
Surface Tension	N/A	
Conductivity	N/A	
Miscellaneous Data	N/A	
Solubility	N/A	

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## 10 - Stability and Reactivity

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### STABILITY

Stable: Stable.

Conditions to Avoid: Air. Moisture.

Materials to Avoid: Strong oxidizing agents, Strong bases, Strong acids Mercury/mercury oxides., Halides

### HAZARDOUS DECOMPOSITION PRODUCTS

Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide.

### HAZARDOUS POLYMERIZATION

Hazardous Polymerization: Will not occur

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## 11 - Toxicological Information

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RTECS NUMBER: ES0525000

### ACUTE TOXICITY

LD50

Skin

Rat

1,240 mg/kg

LD50

Skin

Rat

660 mg/kg

LC50

Inhalation

Rat

2,500 mg/m<sup>3</sup>

4 H

LD50

Oral

Rat

105 mg/kg

Remarks: Behavioral:Somnolence (general depressed activity).  
Lungs, Thorax, or Respiration:Respiratory stimulation.  
Blood:Other changes.

LD50

Intraperitoneal

Rat

52435 UG/KG

LD50

Oral

Mouse

105 mg/kg

Remarks: Lungs, Thorax, or Respiration:Respiratory stimulation.  
Behavioral:Somnolence (general depressed activity). Blood:Other  
changes.

LD50

Oral

Rabbit

150 mg/kg

Remarks: Behavioral:Somnolence (general depressed activity).  
Lungs, Thorax, or Respiration:Respiratory stimulation.  
Blood:Other changes.

LD50

Oral

Guinea pig

130 mg/kg

Remarks: Blood:Other changes. Lungs, Thorax, or  
Respiration:Respiratory stimulation. Behavioral:Somnolence  
(general depressed activity).

LD50

Oral

Bird (wild)

75 mg/kg

#### IRRITATION DATA

Skin

Rabbit

Remarks: Moderate irritation effect

Eyes

Rabbit

Remarks: No irritation effect

Eyes

Rabbit

Remarks: Moderate irritation effect

#### SENSITIZATION

Sensitization: Sensitizer.

Skin: May cause allergic skin reaction.

#### SIGNS AND SYMPTOMS OF EXPOSURE

To the best of our knowledge, the chemical, physical, and

toxicological properties have not been thoroughly investigated.  
CNS depression. Narcotic effect. Prolonged exposure can cause:

#### ROUTE OF EXPOSURE

Skin Contact: Causes burns.

Skin Absorption: Harmful if absorbed through skin.

Eye Contact: Causes burns.

Inhalation: Toxic if inhaled. Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.

Ingestion: Toxic if swallowed.

#### CHRONIC EXPOSURE - REPRODUCTIVE HAZARD

Species: Rat

Dose: 880 MG/KG

Route of Application: Oral

Exposure Time: (5-15D PREG)

Result: Maternal Effects: Other effects.

Species: Rat

Dose: 800 MG/KG

Route of Application: Oral

Exposure Time: (6-15D PREG)

Result: Specific Developmental Abnormalities: Musculoskeletal system. Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus). Maternal Effects: Other effects.

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#### 12 - Ecological Information

N/A

#### ECOTOXICOLOGICAL EFFECTS

Test Type: LC50 Fish

Species: Pimephales promelas (Fathead minnow)

Time: 96 h

Value: 53.6 mg/l

Test Type: EC50 Daphnia

Species: Daphnia magna

Time: 48 h

Value: 26.8 mg/l

Test Type: EC50 Algae

Species: Scenedesmus subspicatus

Time: 72 h

Value: 480 mg/l

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#### 13 - Disposal Considerations

#### SUBSTANCE DISPOSAL

Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations.

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#### 14 - Transport Information

RID/ADR

UN#: 2716

Class: 6.1

PG: III  
Proper Shipping Name: 1,4-Butynediol

IMDG

UN#: 2716  
Class: 6.1  
PG: III  
Proper Shipping Name: 1,4-Butynediol  
Marine Pollutant: No  
Severe Marine Pollutant: No

IATA

UN#: 2716  
Class: 6.1  
PG: III  
Proper Shipping Name: 1,4-Butynediol  
Inhalation Packing Group I: No

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15 - Regulatory Information

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CLASSIFICATION AND LABELING ACCORDING TO EU DIRECTIVES

ANNEX I INDEX NUMBER: 603-076-00-9

INDICATION OF DANGER: T-C

Toxic. Corrosive.

R-PHRASES: 21-23/25-34-43-48/22

Harmful in contact with skin. Toxic by inhalation and if swallowed. Causes burns. May cause sensitization by skin contact. Harmful: danger of serious damage to health by prolonged exposure if swallowed.

S-PHRASES: 25-26-36/37/39-45-46

Avoid contact with eyes. In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing, gloves, and eye/face protection. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). If swallowed, seek medical advice immediately and show this container or label.

COUNTRY SPECIFIC INFORMATION

Germany

WGK: 2  
ID-Number: 1149  
KBwS-Decision

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16 - Other Information

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WARRANTY

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 Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale. Copyright 2008 Sigma-Aldrich Co. License granted to make unlimited paper copies for internal use only.

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