



# Target Molecules

Creation Date:	May 21, 2024
Revision Date:	May 21, 2024

# According to the UN GHS revision 8

1.	IDENTIFICATION		
1.1	GHS Product identifier		
	Product name: 📀	1,3-BUTANEDIOL	
	Catalog Number:	T9257	
	CAS Number:	107-88-0	
1.2	Other means of identifica	ation	
	Other names:	-	
1.3	Recommended use of the	e chemical and restrictions on use	
	Identified uses:		
1.4	Supplier's details		
	Company:	Targetmol Chemicals Inc.	
	Uses advised against:	36 Washington Street,Wellesley Hills, Massachusetts 02481 USA	
	Tel/Fax:	(781) 999-4286	
1.5	Emergency phone numbe	er	
	Emergency phone number:	781-999-4286	
	Service hours:	Monday to Friday, 9am-5pm (Standard timezone:UTC/GMT -5hours).	
2.	HAZARD IDENTIFICATION		
2.1	I Classification of the substance or mixture		
	Not classified.		
2.2	GHS label elements, inclu	uding precautionary statements	
	Pictogram(s):		
	Signal word:	No signal word	
	Hazard statement(s):	none	
	Precautionary statement(s):		
	Prevention:	none	
	Response:	none	
	Storage:	none	
	Disposal:	none	
2.3	Other hazards which do r	not resultin classification	
	no data available		
3.	COMPOSITION/INFORMAT	TION ON INGREDIENTS	
3.1	Substances		

# A DRUG SCREENING EXPERT

Chemical name	Common names and synonyms	CAS number	EC number
1,3-BUTANEDIOL	-	107-88-0	203-529-7

## 4. FIRST-AID MEASURES

## 4.1 Description of necessary first-aid measures

## General advice

no data available

## If inhaled

Fresh air, rest.

## Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap.

## Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

## Following ingestion

Rinse mouth. Give one or two glasses of water to drink. Rest.

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

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Higher alcohols (> 3 carbons) and related compounds

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

no data available

## 5. FIRE-FIGHTING MEASURES

## 5.1 Extinguishing media

Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

## 5.2 Specific hazards arising from the chemical

Combustible.

## 5.3 Special protective actions for fire-fighters

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

## 6. ACCIDENTAL RELEASE MEASURES

## 6.1 Personal precautions, protective equipment and emergency procedures

Collect leaking and spilled liquid in sealable containers as far as possible. Wash away remainder with plenty of water.

## 6.2 Environmental precautions

Collect leaking and spilled liquid in sealable containers as far as possible. Wash away remainder with plenty of water.

## 6.3 Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous wast. Keep in suitable, closed containers for disposal.

## 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

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

## 8.1 Control parameters

Occupational Exposure limit values

no data available

**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 riskelimination area.

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

#### Eye/face protection

Wear safety spectacles.

#### **Skin protection**

Protective gloves.

### **Respiratory protection**

Use ventilation.

## Thermal hazards

no data available

## 9. PHYSICAL AND CHEMICAL PROPERTIES

Physical state	Liquid
Color	Viscous liquid
Odour	Practically odorless
Melting point/ freezing point	172°C(lit.)
Boilingpoint or initial boiling point and boiling range	203-204°C(lit.)
Flammability	Combustible.
Lower and upper explosion limit/flammability limit	no data available
Flash point	108°C
Auto-ignition temperature	741°F
Decomposition temperature	no data available
рН	no data available
Kinematic viscosity	96 cSt at 25 deg C
Solubility	DMSO: 60 mg/ml (665.78 mM)
N-octanol-water partition coefficient	log Kow = -0.29 (est)

## A DRUG SCREENING EXPERT

Vapour pressure	0.0541mmHg at 25°C
Density and/ or relative density	1.005g/mLat 25°C(lit.)
Relative vapour density	3.1 (20 °C, vs air)
Particle characteristics	no data available

## **10. STABILITY AND REACTIVITY**

## 10.1 Reactivity

no data available 🤇

## 10.2 Chemical stability

no data available

## 10.3 Possibility of hazardous reactions

Combustible when exposed to heat or flame.

## 10.4 Conditions to avoid

no data available

## 10.5 Incompatible materials

Incompatible with oxidizing materials.

## 10.6 Hazardous decomposition products

When heated to decomposition it emits acrid smoke and irritating fumes.

## 11. TOXICOLOGICAL INFORMATION

### Acute toxicity

Oral: LD50 Rat oral 22800 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

The substance is irritating to the eyes, skin and respiratory tract.

STOT-repeated exposure

no data available

## Aspiration hazard

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20°C.

## 12. ECOLOGICAL INFORMATION

## 12.1 Toxicity

Toxicity to fish: no data available Toxicity to daphnia and other aquatic invertebrates: no data available Toxicity to algae: no data available Toxicity to microorganisms: no data available

## 12.2 Persistence and degradability

AEROBIC: 1,3-Butanediol was biodegraded 80.5% in 28 days using an unacclimated domestic sludge and the modified Sturm test (OECD 301B)(1). 1,3-Butanediol was found to be readily biodegradable(2). Other pure culture screening studies have demonstrated that 1,3-butanediol can be biodegraded(3-6).

## 12.3 Bioaccumulative potential

An estimated BCF of 3 was calculated in fish for 1,3-butanediol(SRC), using an estimated log Kow of -0.29(1) and a regression-derived equation(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is low (SRC).

## 12.4 Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of 1,3-butanediol can be estimated to be 1(SRC). According to a classification scheme(2), this estimated Koc value suggests that 1,3-butanediol is expected to have very high mobility in soil.

## 12.5 Other adverse effects

no data available

## 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.

## 14. TRANSPORT INFORMATION

## 14.1 UN Number

no data available

## 14.2 UN Proper Shipping Name

no data available

## 14.3 Transport hazard class(es)

no data available

## 14.4 Packing group, if applicable

no data available 🛛 🤇

## 14.5 Environmental hazards

no data available

## 14.6 Special precautions for user

no data available

## 14.7 Transport in bulk according to IMO instruments

no data available

## **15. REGULATORY INFORMATION**

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

Listed.
Listed.
Listed.
Not Listed.
Listed.
Listed.
Listed.
Listed.
Listed.

## 16. OTHER INFORMATION

#### Information on revision

Creation Date	May 21, 2024
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#### 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**

no data available

Disclaimer: 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. We as supplier shall not be held liable for any damage resulting from handling or from contact with the above product. All products are for Research Use Only · Not For Human or Veterinary or Therapeutic Use