

# SAFETY DATA SHEETS

According to the UN GHS revision 10

## 1: Identification

### 1.1 GHS Product identifier

**Product name** 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate

### 1.2 Other means of identification

**Product number** 6846-50-0

**Other names** 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate

### 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** Zhongshan Greenrock Technology Co., Ltd.

**Address** No. 138, Jinsan Avenue, Sanjiao Town, Zhongshan City, Guangdong Province, China

**Telephone** +86-2087066781

### 1.5 Emergency phone number

**Emergency phone number** +86-2087066781

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

## 2: Hazard identification

### 2.1 Emergency Overview

Substances with long-term health risks may cause cancer, gene mutations, or reproductive system damage. Even short-term exposure may have long-term health effects and exposure must be strictly controlled.

### 2.2 GHS Classification

Reproductive toxicity : Category 2

Hazardous to the aquatic environment, long-term hazard : Category 3

### 2.3 GHS label elements, including precautionary statements

**Pictogram(s)****Signal word**

Warning

**Hazard statement(s)**H361 Suspected of damaging fertility or the unborn child  
H412 Harmful to aquatic life with long lasting effects**Precautionary statement(s)****Prevention**P203 Obtain, read and follow all safety instructions before use.  
P273 Avoid release to the environment.  
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...**Response**

P318 if exposed or concerned, get medical advice.

**Storage**

P405 Store locked up.

**Disposal**

P501 Dispose of contents/container to ...

## 2.4 Physical and chemical

Although they may not be immediately dangerous, some substances may also be irritants or corrosives. They may decompose and produce more toxic products during long-term storage.

## 2.5 Health hazards

Carcinogenicity, Long-term exposure may increase the risk of cancer. Mutagenicity: May cause genetic damage, affecting offspring. Reproductive toxicity: May affect fertility or cause fetal malformations. Symptoms typically appear after a latent period of several years.

## 2.6 Environmental hazards

May persist and accumulate in the environment. Chronic toxicity to aquatic and terrestrial organisms can affect their reproductive capacity. It may accumulate through the food chain, ultimately affecting human health.

## 2.7 Other hazards which do not result in classification

no data available

# 3: Composition/information on ingredients

## 3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	6846-50-0	229-934-9	99%

## 4: First-aid measures

### 4.1 General advice

Stop contact immediately and remove contaminated clothing (rinse with clean water and then wash); wash skin with soap and water, record contact history (including contact time and frequency); and have regular physical examinations (such as chest CT and blood routine once a year).

### 4.2 If inhaled

Move to fresh air. If carcinogenic gases (such as benzene) are inhaled and coughing or chest tightness occurs, seek medical attention. Those with long-term exposure need to monitor lung function and blood routine.

### 4.3 In case of skin contact

Rinse with soap and running water for 15 minutes. If skin is irritated, apply a non-irritating moisturizer; avoid breaking the skin to prevent penetration of substances.

### 4.4 In case of eye contact

Rinse with saline for 10 minutes and then instill artificial tears; if discomfort persists, seek medical attention from an ophthalmologist.

### 4.5 If swallowed

Do not induce vomiting, seek medical attention immediately, and bring the substance's SDS; inform the doctor of the substance's carcinogenic/mutagenic properties and perform a gastrointestinal endoscopy if necessary.

### 4.6 Most important symptoms and effects, both acute and delayed

Acute symptoms: mild skin/eye irritation; long-term effects: carcinogenicity (such as lung cancer, leukemia), mutagenicity (chromosomal abnormalities), reproductive toxicity (infertility, fetal malformations).

### 4.7 Protection of first-aiders

Rescuers need to wear chemical protective clothing, gas masks (equipped with organic vapor filter cartridges), and chemical protective gloves; equipment must be thoroughly cleaned after contact to avoid residue.

### 4.8 Notes to physician

Inform the doctor of the substance name and exposure history; long-term exposure requires a special physical examination plan (such as blood tests every 6 months and tumor markers every year)

## 5: Fire-fighting measures

### 5.1 Unsuitable extinguishing media

It is strictly forbidden to use fire extinguishing agents that may cause the spread of toxic substances (such as high-pressure water jets); if it contains flammable ingredients, avoid using carbon dioxide (concentrated toxic vapor).

## **5.2 Specific hazards during fire fighting**

Combustion releases carcinogenic/mutagenic gases (such as benzopyrene and formaldehyde), which are harmful to health if exposed for a long time. The combustion products of some substances are easily adsorbed on dust, expanding the scope of pollution. Toxic substances are not easy to decompose and require professional handling after fire extinguishing.

## **5.3 Hazardous combustion products**

Polycyclic aromatic hydrocarbons (carcinogenic), formaldehyde (mutagenic), heavy metal smoke (such as chromium, nickel), chlorides (when containing chlorine).

## **5.4 Specific extinguishing methods**

Small area: Use dry powder/foam to extinguish the fire, and use water mist to dilute the toxic vapor; Large area: Evacuate personnel, if fire must be extinguished, cover with foam (to reduce vapor release); After extinguishing the fire, conduct toxicity testing on the area and dispose of pollutants as hazardous waste.

## **5.5 Special protective equipment for fire-fighters**

Wear chemical protective clothing, positive pressure air respirator, and chemical protective gloves; carry a toxic gas detector (to detect benzene, formaldehyde, etc.); wear a dust mask (to protect against toxic dust) during work, and conduct a health check after work.

# **6: Accidental release measures**

## **6.1 Protective measures for workers**

Wear fully enclosed chemical protective clothing, positive pressure respirator (volatile), toxic-resistant gloves + goggles; workers should undergo regular physical examinations and record their exposure history; eating, drinking and smoking are prohibited.

## **6.2 Environmental protection measure**

Isolate the contaminated area within 20 meters and conduct long-term environmental monitoring (soil/air); leaks are prohibited from being discarded at will; the contaminated area must be released after passing the inspection by the environmental protection department.

## **6.3 Containment methods for leaked chemicals**

Liquids should be collected in disposable corrosion-resistant containers (marked with hazard categories); solids should be collected in chemical-resistant bags (to prevent dust); and stored separately in dedicated hazardous waste warehouses.

## **6.4 Cleanup methods for chemical spills**

Small leakage: absorbed by special adsorption materials and then packaged in chemical-proof bags; large leakage: transferred by professional team using special equipment; after cleaning, the ground is treated with disinfectant.

## 6.5 Measures to prevent the spread of leaks

20-meter isolation zone + warning signs; high-efficiency filtration and ventilation (volatile); chemical isolation belt to prevent spread to residential areas.

## 6.6 Container leakage treatment

Minor leaks: seal with professional sealant + tightness test; serious leaks: evacuate, transfer by professional team, and dispose of the container as hazardous waste.

## 6.7 Special considerations

Operators need special training; protective equipment must be disinfected and tested before reuse; leak handling must be reported to the environmental protection department.

# 7: Handling and storage

## 7.1 Safe storage conditions

Stored in a closed, leak-proof warehouse (walls lined with polyethylene film and floors with impermeable resin); containers are made of non-degradable materials (such as high-density polyethylene, borosilicate glass) with anti-theft lids (requires a key to open); the warehouse is equipped with an air purification system (HEPA filter, filtration efficiency >99.97%).

## 7.2 Storage precautions

Isolate from children and unrelated personnel, and place biohazard signs at the warehouse entrance; store separately to avoid mixing with other chemicals; test the concentration of hazardous substances in the warehouse every quarter to ensure that it is below the occupational exposure limit (such as carcinogen OEL > 0.01mg/m<sup>3</sup>); discarded containers must be sterilized at high temperature (>121°, 30 minutes) before disposal.

## 7.3 VCI Storage Grade

Level 4 (lowest): Metal containers are treated with ordinary anti-rust treatment (such as galvanizing, thickness > 10µm) and corrosion is checked once a year; the humidity in the warehouse is controlled at 45%-65% to avoid damage to the containers due to moisture.

## 7.4 Recommended storage temperature

Store at 10-30°C, away from light (e.g., some photosensitive carcinogens must be stored in brown containers); easily degradable substances (e.g., some organic carcinogens) must be stored at >25°C, equipped with light-proof and sun-shading facilities; long-term storage (over 1 year) requires the stability of the substance to be checked every 3 months (if the label has a recommended storage temperature, follow the label).

## 7.5 Handling

For precautions see Safety Data Sheet section 2

Advice on safe handling : Work under hood. Do not inhale substance/mixture.

## 8: Exposure controls/personal protection

### 8.1 Respiratory protection

When exposed to carcinogens (such as benzene and formaldehyde) for a long time, wear a powered air-purifying respirator (APF?50); dust (such as asbestos) requires Type P100 filter cotton to ensure no leakage.

### 8.2 Recommended Filter type

For organic carcinogens, choose Type A2 filter cartridge; for inorganic carcinogenic gases (such as arsine), choose Type E+K composite filter cartridge; for dust, choose Type P100 filter cotton.

### 8.3 Eye/face protection

Wear chemical protection goggles + protective mask. The mask material should be resistant to toxic penetration. The lenses need to be replaced regularly for long-term work (to prevent aging).

### 8.4 Skin and body protection

Wear impermeable chemical protective clothing made of polyethylene + aluminum foil coating (anti-organic vapor penetration); avoid skin damage during operation to prevent material intrusion.

### 8.5 Hand protection

Wear toxic and chemical-resistant gloves made of butyl rubber or fluororubber. Gloves need to be regularly tested for penetration (once every three months) and replaced immediately if unqualified.

### 8.6 Hygiene measures

After work, clean the skin with a special detergent (such as a neutral surfactant), then rinse with running water for 10 minutes; clothes must be washed separately and must not be mixed with household clothes; undergo special physical examinations every year (such as chest CT, chromosome examination).

## 9: Physical and chemical properties and safety characteristics

<b>Physical state</b>	CLEAR COLORLESS LIQUID
<b>Colour</b>	Low color
<b>Odour</b>	no data available
<b>Melting point/freezing point</b>	-70°C(lit.)
<b>Boiling point or initial boiling point and boiling range</b>	280°C(lit.)
<b>Flammability</b>	no data available
<b>Lower and upper explosion limit/flammability limit</b>	Lower flammable limit: 0.5% by volume at 342 deg F (172°C)

<b>Flash point</b>	121°C(lit.)
<b>Auto-ignition temperature</b>	795 deg F (424°C)
<b>Decomposition temperature</b>	When heated to decomposition it emits acrid smoke and irritating fumes.
<b>pH</b>	no data available
<b>Kinematic viscosity</b>	no data available
<b>Solubility</b>	In water, 11.4 mg/L at 25°C (est)
<b>Partition coefficient n-octanol/water</b>	log Kow = 4.91 (est)
<b>Vapour pressure</b>	8.5X10-3 mm Hg at 25°C (est)
<b>Density and/or relative density</b>	0.941 g/mL at 25oC(lit.)
<b>Relative vapour density</b>	9.9 (Air = 1)
<b>Particle characteristics</b>	no data available

## 10: Stability and reactivity

### 10.1 Reactivity

no data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

no data available

### 10.4 Conditions to avoid

no data available

### 10.5 Incompatible materials

no data available

### 10.6 Hazardous decomposition products

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

## 11: Toxicological information

### 11.1 Acute toxicity

Oral: LD50 Mouse oral >6400 mg/kg bw  
Inhalation: LC50 Rat inhalation >5.3 mg/L 6hr  
Dermal: no data available

### 11.2 Skin corrosion/irritation

no data available

### 11.3 Serious eye damage/irritation

no data available

### 11.4 Respiratory or skin sensitization

no data available

### 11.5 Germ cell mutagenicity

no data available

### 11.6 Carcinogenicity

no data available

### 11.7 Reproductive toxicity

no data available

### 11.8 STOT-single exposure

no data available

### 11.9 STOT-repeated exposure

no data available

### 11.10 Aspiration hazard

no data available

## 12: Ecological information

### 12.1 Toxicity

Toxicity to fish: LC50; Species: Pimephales promelas (Fathead minnow); Conditions: freshwater, static;  
Concentration: >1.55 mg/L for 96 hr  
Toxicity to daphnia and other aquatic invertebrates: LC50; Species: Daphnia magna (Water flea);  
Conditions: static; Concentration: 300 mg/L for 24 hr /from table  
Toxicity to algae: no data available

Toxicity to microorganisms: no data available

## 12.2 Persistence and degradability

Biodegradation data for 2,2,4-trimethyl-1,3-pentanediol in soil or water were not available. (SRC, 2012)

## 12.3 Bioaccumulative potential

An estimated BCF of 800 was calculated in fish for 2,2,4-trimethyl-1,3-pentanediol diisobutyrate(SRC), using an estimated log Kow of 4.91(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is high(SRC), provided the compound is not metabolized by the organism(SRC).

## 12.4 Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of 2,2,4-trimethyl-1,3-pentanediol diisobutyrate can be estimated to be 490(SRC). According to a classification scheme(2), this estimated Koc value suggests that 2,2,4-trimethyl-1,3-pentanediol diisobutyrate is expected to have low mobility in soil. 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate concentrations were 500 and 120 ng/L in influent and effluent, respectively, using a soil column test and secondary treated City of Phoenix, AZ wastewater; the decrease in effluent was attributed mainly to adsorption(3).

## 12.5 Other adverse effects

no data available

# 13: Disposal considerations

## 13.1 Disposal methods for waste chemicals

It must be handled by an organization with hazardous waste disposal qualifications, with high-temperature incineration (temperature ? 900°C) being preferred to completely destroy hazardous substances. Waste that cannot be incinerated must be chemically degraded or stabilized before being safely landfilled. Contaminated containers must be sterilized at high temperatures or chemically before disposal.

## 13.2 Precautions

Disposal personnel must wear special protective equipment and undergo regular health checks; waste must be tightly sealed to prevent leakage; waste gas and wastewater generated during the disposal process must undergo special treatment to ensure compliance with standards; disposal records must be kept for a long time (at least 30 years); and mixing with ordinary waste is prohibited.

# 14: Transport information

## 14.1 UN Number

ADR/RID: UN2734

IMDG: UN2734

IATA: UN2734

## 14.2 UN Proper Shipping Name

ADR/RID: AMINES, LIQUID,  
CORROSIVE, FLAMMABLE,  
N.O.S. or POLYAMINES,  
LIQUID, CORROSIVE,  
FLAMMABLE, N.O.S.

IMDG: AMINES, LIQUID,  
CORROSIVE, FLAMMABLE,  
N.O.S. or POLYAMINES,  
LIQUID, CORROSIVE,  
FLAMMABLE, N.O.S.

IATA: AMINES, LIQUID,  
CORROSIVE, FLAMMABLE,  
N.O.S. or POLYAMINES,  
LIQUID, CORROSIVE,  
FLAMMABLE, N.O.S.

### 14.3 Transport hazard class(es)

ADR/RID: 8

IMDG: 8

IATA: 8

### 14.4 Packing group, if applicable

ADR/RID: II

IMDG: II

IATA: II

### 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

## 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
2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	6846-50-0	229-934-9
New Zealand Inventory of Chemicals (NZIoC)			Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Listed.
Australian Inventory of Industrial Chemicals (AIIC)			Not Listed.
Catalogue of Strictly Restricted Toxic Chemicals in China			Not Listed.
China Catalog of Hazardous chemicals 2015			Not Listed.
European INventory of Existing Commercial chemical Substances			Not Listed.
IARC Monographs on the Evaluation of Carcinogenic Risks to Humans			Not Listed.
TSCA Inventory of Chemical Substances			Listed.

## 16: Other information

## Information on revision

SDS Creation Date July 1, 2025

SDS Revision Date July 1, 2025

## Abbreviations and acronyms in SDS

- 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%

## SDS 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/>

**Any questions regarding this Safety Data Sheet, Please send your inquiry to [sales@MolBest.com](mailto:sales@MolBest.com)**

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