

# • SAFETY DATA SHEET

Version 7.0  
Revision Date 03/16/2026  
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## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

Product name : 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate  
Product Number : 525170  
Brand : Aldrich  
CAS-No. : 6846-50-0

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

Identified uses : Laboratory chemicals, Synthesis of substances  
Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

### 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES  
Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

### 1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

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## SECTION 2. HAZARDS IDENTIFICATION

**GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)**

**Hazards for the product as supplied**

Reproductive toxicity : Category 2

Long-term (chronic) aquatic hazard : Category 3

### Other hazards

None known.

### GHS label elements

Hazard pictograms :



Signal word : Warning

Hazard statements : H361 Suspected of damaging fertility or the unborn child.  
H412 Harmful to aquatic life with long lasting effects.

Precautionary statements : **Prevention:**  
P201 Obtain special instructions before use.  
P202 Do not handle until all safety precautions have been read and understood.  
P273 Avoid release to the environment.  
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.  
**Response:**  
P308 + P313 IF exposed or concerned: Get medical advice/ attention.  
**Storage:**  
P405 Store locked up.  
**Disposal:**  
P501 Dispose of contents/ container to an approved waste disposal plant.

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## SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 6846-50-0

### Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
1-Isopropyl-2,2-dimethyltrimethylene diisobutyrate	6846-50-0*	>= 80 - <= 100	TSC

\* Indicates that the identifier is a CAS No.

TSC- the actual concentration or concentration range is withheld as a trade secret

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#### SECTION 4. FIRST AID MEASURES

- General advice : Show this safety data sheet to the doctor in attendance.
- If inhaled : After inhalation: fresh air. Call in physician.
- In case of skin contact : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.
- In case of eye contact : After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.
- If swallowed : After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.
- Most important symptoms and effects, both acute and delayed : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11
- Protection of first-aiders : For personal protection see section 8.
- Notes to physician : No data available

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#### SECTION 5. FIREFIGHTING MEASURES

- Suitable extinguishing media : Foam  
Carbon dioxide (CO<sub>2</sub>)  
Dry powder
- Unsuitable extinguishing media : For this substance/mixture no limitations of extinguishing agents are given.
- Specific hazards during fire fighting : Combustible.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

- Hazardous combustion products : Carbon oxides
- Specific extinguishing methods : No data available
- Further information : Prevent fire extinguishing water from contaminating surface water or the ground water system.
- Special protective equipment for fire-fighters : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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## SECTION 6. ACCIDENTAL RELEASE MEASURES

- Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:  
Do not breathe vapours, aerosols.  
Avoid substance contact.  
Ensure adequate ventilation.  
Evacuate the danger area, observe emergency procedures, consult an expert.  
Advice for emergency responders:  
For personal protection see section 8.
- Environmental precautions : Do not let product enter drains.
- Methods and materials for containment and cleaning up : Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10).  
Take up with liquid-absorbent material (e.g. Chemizorb® ). Dispose of properly. Clean up affected area.

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

- Further information on storage conditions : Tightly closed.  
Keep locked up or in an area accessible only to

qualified or authorised persons.

Storage class : 10, Combustible liquids

Recommended storage temperature : Recommended storage temperature see product label.

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## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

**Engineering measures** : No data available

### Personal protective equipment

Respiratory protection : required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

### Hand protection

Material : Nitrile rubber  
Break through time : 10 min  
Glove thickness : 0.11 mm  
Protective index : Splash contact  
Manufacturer : Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Material : Nitrile rubber  
Break through time : 480 min  
Glove thickness : 0.4 mm  
Protective index : Full contact  
Manufacturer : Camatril® (KCL 730 / Aldrich Z677442, Size M)

Remarks : This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the

supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

- Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).  
Safety glasses
- Skin and body protection : protective clothing
- Hygiene measures : Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

- Appearance : liquid
- Color : colourless
- Odor : No data available
- Odor Threshold : No data available  
pH : No data available
- Melting point/ range : -94 °F / -70 °C  
Method: lit.
- Boiling point/boiling range : 536 °F / 280 °C (1,013 hPa)
- Flash point : 277 °F / 136 °C  
(1013.250 hPa)  
Method: closed cup, Non-equilibrium method
- Evaporation rate : No data available
- Flammability (solid, gas) : No data available
- Flammability (liquids) : No data available
- Burning rate : No data available
- Self-ignition : 748 °F / 398 °C  
98 kPa
- Upper explosion limit /  
Upper flammability limit : Upper flammability limit  
3.1 %(V)

Aldrich - 525170

Page 6 of 14

Lower explosion limit / Lower flammability limit	: ( 446 °F / 230 °C) Lower flammability limit 0.48 %(V)
Vapor pressure	: ( 342 °F / 172 °C) < 1 hPa (77 °F / 25 °C) Method: OECD Test Guideline 104
Relative vapour density	: No data available
Relative density	: No data available
Density	: 0.941 g/cm <sup>3</sup>
Solubility(ies) Water solubility	: 0.0127 g/l slightly soluble (81.5 °F / 27.5 °C) pH: 3.6 - 4.6
Partition coefficient: n- octanol/water	: log Pow: 4.9 (77 °F / 25 °C) Method: EPI Suite™ Potential bioaccumulation (Lit.)
Autoignition temperature	: 795 °F / 424 °C
Decomposition temperature	: No data available
Viscosity Viscosity, dynamic	: 5.04 mPa.s (77 °F / 25 °C) Method: OECD Test Guideline 114
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: none
Surface tension	: 27.8 mN/m, 72 °F / 22 °C, OECD Test Guideline 115
Molecular weight	: 286.41 g/mol
Particle characteristics Particle size	: No data available

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## SECTION 10. STABILITY AND REACTIVITY

Reactivity : Forms explosive mixtures with air on intense heating.  
A range from approx. 15 Kelvin below the flash point

Aldrich - 525170

Page 7 of 14

The life science business of Merck KGaA, Darmstadt, Germany  
operates as MilliporeSigma in the US and Canada

**MILLIPORE  
SIGMA**

is to be rated as critical.

- Chemical stability : The product is chemically stable under standard ambient conditions (room temperature) .
- Possibility of hazardous reactions : No data available
- Conditions to avoid : Strong heating.
- Incompatible materials : Strong oxidizing agents
- Hazardous decomposition products : In the event of fire: see section 5

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## SECTION 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - female - > 2,000 mg/kg

(OECD Test Guideline 425)

Inhalation: No data available

LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg

(OECD Test Guideline 402)

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Aldrich - 525170

Page 8 of 14

Result: negative

### **Carcinogenicity**

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

### **Reproductive toxicity**

Suspected of damaging the unborn child.

### **Specific target organ toxicity - single exposure**

No data available

### **Specific target organ toxicity - repeated exposure**

No data available

### **Aspiration hazard**

No data available

## **11.2 Additional Information**

RTECS: SA1420000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## **SECTION 12. ECOLOGICAL INFORMATION**

### **Ecotoxicity**

#### **Components:**

#### **1-Isopropyl-2,2-dimethyltrimethylene diisobutyrate:**

Toxicity to fish : NOEC (Lepomis macrochirus):  $\geq 6$  mg/l  
Exposure time: 96 h  
Test Type: flow-through test  
Analytical monitoring: yes  
Method: OECD Test Guideline 203  
GLP: yes

Toxicity to algae/aquatic plants : ErC50 (Pseudokirchneriella subcapitata (green algae)):  $> 7.49$  mg/l  
Exposure time: 72 h  
Test Type: Growth inhibition  
Analytical monitoring: yes  
Method: OECD Test Guideline 201  
GLP: yes

NOEC (Pseudokirchneriella subcapitata (green algae)):  
3.56 mg/l

Exposure time: 72 h  
Test Type: Growth inhibition  
Analytical monitoring: yes  
Method: OECD Test Guideline 201  
GLP: yes

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity) : NOEC (Daphnia magna (Water flea)): 0.7 mg/l  
End point: reproduction rate  
Exposure time: 21 d  
Test Type: flow-through test  
Analytical monitoring: yes  
Method: OECD Test Guideline 211  
GLP: yes

### **Ecotoxicology Assessment**

Chronic aquatic toxicity : Harmful to aquatic life with long lasting effects.

### **Persistence and degradability**

#### **Components:**

#### **1-Isopropyl-2,2-dimethyltrimethylene diisobutyrate:**

Biodegradability : aerobic  
Inoculum: activated sludge  
Concentration: 10 mg/l  
Result: Readily biodegradable.  
Biodegradation: 70.73 %  
Exposure time: 28 d  
Method: OECD Test Guideline 301B  
GLP: yes  
Remarks: The 10 day time window criterion is not fulfilled.

### **Bioaccumulative potential**

#### **Components:**

#### **1-Isopropyl-2,2-dimethyltrimethylene diisobutyrate:**

Partition coefficient: n-octanol/water : log Pow: 4.9 (77 °F / 25 °C)  
Method: EPI Suite™  
Remarks: Potential bioaccumulation (Lit.)

### **Mobility in soil**

#### **Components:**

#### **1-Isopropyl-2,2-dimethyltrimethylene diisobutyrate:**

Stability in soil : Remarks: No data available

## Other adverse effects

### Product:

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances  
Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

### Components:

#### **1-Isopropyl-2,2-dimethyltrimethylene diisobutyrate:**

Additional ecological information : No data available

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## SECTION 13. DISPOSAL CONSIDERATIONS

### **Disposal methods**

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## SECTION 14. TRANSPORT INFORMATION

### **International Regulations**

#### **IATA-DGR**

Not regulated as a dangerous good

#### **IMDG-Code**

Not regulated as a dangerous good

#### **Transport in bulk according to IMO instruments**

Not applicable for product as supplied.

### **National Regulations**

#### **49 CFR Road**

Not regulated as a dangerous good

Poison Inhalation Hazard : No

### **Special precautions for user**

Remarks : Not classified as dangerous in the meaning of transport regulations.

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## SECTION 15. REGULATORY INFORMATION

### **CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

### **SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

### **SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : No SARA Hazards

**SARA 313** : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

### **Clean Air Act**

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCOMI Intermediate or Final VOC's (40 CFR 60.489).

### **Clean Water Act**

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

### **US State Regulations**

#### **Massachusetts Right To Know**

No components are subject to the Massachusetts Right to Know Act.

#### **Maine Chemicals of High Concern**

Product does not contain any listed chemicals

#### **Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

#### **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

### **The components of this product are reported in the following inventories:**

US TSCA : All substances listed as active on the TSCA inventory

### **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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## **SECTION 16. OTHER INFORMATION**

### **Relevant changes since previous version**

8. Exposure controls/personal protection

### **Full text of other abbreviations**

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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