

## SAFETY DATA SHEET

Version 4.5  
Revision Date 04/24/2018  
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**1. PRODUCT AND COMPANY 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

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

Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

**1.4 Emergency telephone number**

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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**2. HAZARDS IDENTIFICATION****2.1 Classification of the substance or mixture**

Not a hazardous substance or mixture.

**2.2 GHS Label elements, including precautionary statements**

Not a hazardous substance or mixture.

**2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none**

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**3. COMPOSITION/INFORMATION ON INGREDIENTS****3.1 Substances**

Synonyms : TXIB

Formula : C<sub>16</sub>H<sub>30</sub>O<sub>4</sub>

Molecular weight : 286.41 g/mol

CAS-No. : 6846-50-0

EC-No. : 229-934-9

No components need to be disclosed according to the applicable regulations.

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## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Flush eyes with water as a precaution.

#### If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 4.2 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

### 4.3 Indication of any immediate medical attention and special treatment needed

No data available

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## 5. FIREFIGHTING MEASURES

### 5.1 Extinguishing media

#### Suitable extinguishing media

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

### 5.2 Special hazards arising from the substance or mixture

No data available

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

No data available

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## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas.  
For personal protection see section 8.

### 6.2 Environmental precautions

Do not let product enter drains.

### 6.3 Methods and materials for containment and cleaning up

Keep in suitable, closed containers for disposal.

### 6.4 Reference to other sections

For disposal see section 13.

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## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

For precautions see section 2.2.

### 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.  
Storage class (TRGS 510): 10: Combustible liquids

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### Personal protective equipment

##### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

##### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

##### Body Protection

Impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

##### Control of environmental exposure

Do not let product enter drains.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid Colour: colourless
b) Odour	No data available
c) Odour Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: -70 °C (-94 °F) - lit.
f) Initial boiling point and boiling range	280 °C (536 °F) at 1,013 hPa (760 mmHg)
g) Flash point	136 °C (277 °F)
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 3.1 %(V) Lower explosion limit: 0.48 %(V)
k) Vapour pressure	< 0.0 hPa (< 0.0 mmHg) at 25 °C (77 °F)
l) Vapour density	No data available
m) Relative density	0.941 g/cm <sup>3</sup>
n) Water solubility	12.7 mg/l at 27.5 °C (81.5 °F) - slightly soluble

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|---|---------------------------------------|
| o) Partition coefficient: n-octanol/water | No data available                     |
| p) Auto-ignition temperature              | 398 °C (748 °F) at 980 hPa (735 mmHg) |
| q) Decomposition temperature              | No data available                     |
| r) Viscosity                              | No data available                     |
| s) Explosive properties                   | No data available                     |
| t) Oxidizing properties                   | No data available                     |

## 9.2 Other safety information

Surface tension	27.8 mN/m at 22 °C (72 °F)
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## 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

Strong oxidizing agents

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

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

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 sensitisation

No data available

**Germ cell mutagenicity**

Hamster

ovary

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**

No data available

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

Repeated dose toxicity Rat - male - NOAEL : 150 mg/kg

RTECS: SA1420000

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

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**12. ECOLOGICAL INFORMATION****12.1 Toxicity**

Toxicity to fish static test LC50 - Pimephales promelas (fathead minnow) - > 1.55 mg/l - 96 h (OECD Test Guideline 203)

Toxicity to algae Growth inhibition EC50 - Selenastrum capricornutum (green algae) - > 7.49 mg/l - 72 h (OECD Test Guideline 201)

**12.2 Persistence and degradability**

Biodegradability aerobic - Exposure time 28 d  
Result: 70.73 % - Readily biodegradable.  
(OECD Test Guideline 301B)  
Remarks: The 10 day time window criterion is not fulfilled.

**12.3 Bioaccumulative potential**

No data available

**12.4 Mobility in soil**

No data available

**12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

**12.6 Other adverse effects**

No data available

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## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

**Product**

Offer surplus and non-recyclable solutions to a licensed disposal company.

**Contaminated packaging**

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

**DOT (US)**

Not dangerous goods

**IMDG**

Not dangerous goods

**IATA**

Not dangerous goods

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## 15. REGULATORY INFORMATION

**SARA 302 Components**

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

**SARA 313 Components**

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.

**SARA 311/312 Hazards**

No SARA Hazards

**Massachusetts Right To Know Components**

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

**Pennsylvania Right To Know Components**

	CAS-No.	Revision Date
1-Isopropyl-2,2-dimethyltrimethylene diisobutyrate	6846-50-0	

**California Prop. 65 Components**

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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## 16. OTHER INFORMATION

**HMIS Rating**

Health hazard:	0
Chronic Health Hazard:	*
Flammability:	1
Physical Hazard	0

**NFPA Rating**

Health hazard:	0
Fire Hazard:	1
Reactivity Hazard:	0

**Further information**

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**Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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