

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 8.0

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : beta,beta,3-Trimethylbenzenepropanol  
 $\beta,\beta,3$ -Trimethylbenzenepropanol  
Product Number : CRM78329  
Brand : Supelco  
Index-No. : 603-138-00-5  
REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.  
CAS-No. : 103694-68-4

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

Identified uses : Laboratory chemicals, Manufacture of substances

### 1.3

CHEMIKART

### 1.4 Emergency telephone

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

#### Classification according to Regulation (EC) No 1272/2008

Long-term (chronic) aquatic hazard (Category 3), H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

### 2.2 Label elements

#### Labelling according Regulation (EC) No 1272/2008

Pictogram : none

Signal Word : none

Hazard statement(s) H412	Harmful to aquatic life with long lasting effects.
Precautionary statement(s) P273	Avoid release to the environment.
P501	Dispose of contents/ container to an approved waste disposal plant.
Supplemental Hazard Statements	none

#### Reduced Labeling (<= 125 ml)

Pictogram none

Signal Word none

Hazard statement(s)  
H412 Harmful to aquatic life with long lasting effects.

Precautionary statement(s)  
none

Supplemental Hazard Statements  
none

### 2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Formula : C<sub>12</sub>H<sub>18</sub>O  
Molecular weight : 178,27 g/mol  
CAS-No. : 103694-68-4  
EC-No. : 687-589-3  
Index-No. : 603-138-00-5

Component		Classification	Concentration
<b>3-(2,2-Dimethyl-3-hydroxypropyl)toluene</b>			
CAS-No.	103694-68-4	Aquatic Chronic 3; H412	<= 100 %
EC-No.	403-140-4		
Index-No.	603-138-00-5		

For the full text of the H-Statements mentioned in this Section, see Section 16.

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### If inhaled

After inhalation: fresh air.

**In case of skin contact**

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

**In case of eye contact**

After eye contact: rinse out with plenty of water. Remove contact lenses.

**If swallowed**

After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

**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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**SECTION 5: Firefighting measures****5.1 Extinguishing media****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.

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

Carbon oxides

Combustible.

Vapors 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.

**5.3 Advice for firefighters**

In the event of fire, wear self-contained breathing apparatus.

**5.4 Further information**

Prevent fire extinguishing water from contaminating surface water or the ground water system.

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**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Evacuate the danger area, observe emergency procedures, consult an expert.

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**

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. Chemisorb® ).

Dispose of properly. Clean up affected area.

## 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 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

#### Storage conditions

Tightly closed.

#### Storage stability

Recommended storage temperature  
-20 °C

Store under argon. Moisture sensitive.

#### Storage class

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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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

### 8.2 Exposure controls

#### 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). Safety glasses

##### Skin protection

not required

##### Respiratory protection

Not required; except in case of aerosol formation.

##### Control of environmental exposure

Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |                                 |                            |
|---------------------------------|----------------------------|
| a) Physical state               | liquid                     |
| b) Color                        | No data available          |
| c) Odor                         | No data available          |
| d) Melting point/freezing point | Melting point/range: 24 °C |

e) Initial boiling point and boiling range	No data available
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	132 °C - closed cup
i) Autoignition temperature	425 °C
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	0,2658 g/l at 25 °C
n) Partition coefficient: n-octanol/water	log Pow: 3,38 at 25 °C
o) Vapor pressure	0,028 hPa at 20 °C
p) Density	0,930 - 0,950 g/cm <sup>3</sup> at 20 °C
Relative density	0,96 at 20 °C
q) Relative vapor density	
r) Particle characteristics	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

## 9.2 Other safety information

Surface tension 43,1 mN/m at 20 °C

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.  
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:  
Strong oxidizing agents

#### 10.4 Conditions to avoid

Strong heating.

#### 10.5 Incompatible materials

No data available

#### 10.6 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

Oral: No data available

Inhalation: No data available

Dermal: No data available

##### Skin corrosion/irritation

No data available

##### Serious eye damage/eye 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

##### 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

##### Endocrine disrupting properties

###### Product:

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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

### 12.1 Toxicity

Toxicity to fish                      flow-through test EC50 - Danio rerio (zebra fish) - 19 mg/l - 96 h  
Remarks: (ECHA)

Toxicity to algae                      static test ErC50 - Desmodesmus subspicatus (green algae) - 27  
mg/l - 72 h  
(OECD Test Guideline 201)

### 12.2 Persistence and degradability

Biodegradability                      Result: 4 % - Not readily biodegradable.  
(OECD Test Guideline 301B)

### 12.3 Bioaccumulative potential

No data available

### 12.4 Mobility in soil

No data available

### 12.5 Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

### 12.6 Endocrine disrupting properties

#### Product:

Assessment                      : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

### 12.7 Other adverse effects

No data available

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### **Product**

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14: Transport information

### 14.1 UN number

ADR/RID: -

IMDG: -

IATA: -

### 14.2 UN proper shipping name

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA: Not dangerous goods

**14.3 Transport hazard class(es)**

ADR/RID: -

IMDG: -

IATA: -

**14.4 Packaging group**

ADR/RID: -

IMDG: -

IATA: -

**14.5 Environmental hazards**

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

**14.6 Special precautions for user****Further information**

Not classified as dangerous in the meaning of transport regulations.

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**SECTION 15: Regulatory information****15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

**Other regulations**

Take note of Dir 94/33/EC on the protection of young people at work.

**15.2 Chemical Safety Assessment**

For this product a chemical safety assessment was not carried out

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**SECTION 16: Other information****Full text of H-Statements referred to under sections 2 and 3.**

H412 Harmful to aquatic life with long lasting effects.

**Further information**

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 Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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