

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 21.01.2015

Version 7.2

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

### 1.1 Product identifier

Catalogue No.	814442
Product name	3,3,5-Trimethylcyclohexanol (mixture of cis- and trans- isomers) for synthesis
REACH Registration Number	A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No.	116-02-9

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

Identified uses	Chemical for synthesis Intermediate for use under strictly controlled conditions For additional information on uses please refer to the Merck Chemicals portal ( <a href="http://www.merckgroup.com">www.merckgroup.com</a> ).
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### 1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	LS-QHC * e-mail: <a href="mailto:prodsafe@merckgroup.com">prodsafe@merckgroup.com</a>

### 1.4 Emergency telephone number

Please contact the regional company representation in your country.

## SECTION 2. Hazards identification

### 2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Specific target organ toxicity - single exposure, Category 3, H335

Eye irritation, Category 2, H319

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

Classification (67/548/EEC or 1999/45/EC)

Xi Irritant R36/37

For the full text of the R-phrases mentioned in this Section, see Section 16.

### 2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 814442  
Product name 3,3,5-Trimethylcyclohexanol (mixture of cis- and trans- isomers) for synthesis

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Warning

*Hazard statements*

H319 Causes serious eye irritation.

H335 May cause respiratory irritation.

*Precautionary statements*

Prevention

P262 Do not get in eyes, on skin, or on clothing.

Response

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Reduced labelling (≤125 ml)

*Hazard pictograms*



*Signal word*

Warning

CAS-No. 116-02-9

2.3 Other hazards

None known.

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SECTION 3. Composition/information on ingredients

3.1 Substance

Formula C<sub>9</sub>H<sub>18</sub>O (Hill)  
EC-No. 204-122-7  
Molar mass 142,24 g/mol

**Hazardous components (REGULATION (EC) No 1272/2008)**

*Chemical Name (Concentration)*

CAS-No.	Registration number	Classification
3,3,5-trimethylcyclohexanol (≤ 100 % )		
116-02-9	*)	

Eye irritation, Category 2, H319

Specific target organ toxicity - single exposure, Category 3, H335

\*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

**Hazardous components (1999/45/EC)**

*Chemical Name (Concentration)*

CAS-No.	Classification
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SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 814442  
Product name 3,3,5-Trimethylcyclohexanol (mixture of cis- and trans- isomers) for synthesis

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3,3,5-trimethylcyclohexanol ( $\leq 100\%$ )  
116-02-9 Xi, Irritant; R36/37

For the full text of the R-phrases mentioned in this Section, see Section 16.

### 3.2 Mixture

Not applicable

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## SECTION 4. First aid measures

### 4.1 Description of first aid measures

After inhalation: fresh air.

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

After eye contact: rinse out with plenty of water. Call in ophthalmologist.

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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

irritant effects, Cough, Shortness of breath, Dizziness, agitation, Diarrhoea, Nausea, Vomiting, drowsiness

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

No information available.

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## SECTION 5. Firefighting measures

### 5.1 Extinguishing media

*Suitable extinguishing media*

Water, 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

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.

### 5.3 Advice for firefighters

*Special protective equipment for firefighters*

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

*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: Avoid inhalation of vapours/aerosols or dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No.	814442
Product name	3,3,5-Trimethylcyclohexanol (mixture of cis- and trans- isomers) for synthesis

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Protective equipment 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). Depending on the state of matter, take up with suitable equipment or with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

#### 6.4 Reference to other sections

Indications about waste treatment see section 13.

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### SECTION 7. Handling and storage

#### 7.1 Precautions for safe handling

*Advice on safe handling*

Observe label precautions.

*Hygiene measures*

Change contaminated clothing. Wash hands after working with substance.

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

*Storage conditions*

Tightly closed. Dry.

Recommended storage temperature see product label.

#### 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

#### 8.2 Exposure controls

The product is registered for use under strictly controlled conditions as defined in Article 18(4) of Regulation (EC) No. 1907/2006 (REACH) and must therefore be handled as such. Refer to the industry guidance prepared by Concawe, Cefic and EFCG for advice on the confirmation of strictly controlled conditions

#### Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

#### Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

*Eye/face protection*

Safety glasses

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 814442  
Product name 3,3,5-Trimethylcyclohexanol (mixture of cis- and trans- isomers) for synthesis

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*Hand protection*

full contact:

Glove material: Nitrile rubber  
Glove thickness: 0,11 mm  
Break through time: > 480 min

splash contact:

Glove material: Nitrile rubber  
Glove thickness: 0,11 mm  
Break through time: > 480 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 741 Dermatril® L (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

*Other protective equipment*

protective clothing

*Respiratory protection*

required when dusts/vapours/aerosols are generated.

Recommended Filter type: Filter A-(P2)

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.

**Environmental exposure controls**

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**

Form	crystals
Colour	colourless
Odour	aromatic
Odour Threshold	No information available.
pH	7 at 1,8 g/l 20 °C
Melting point	30 - 32 °C
Boiling point/boiling range	193 - 196 °C at 1.013 hPa

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No.	814442
Product name	3,3,5-Trimethylcyclohexanol (mixture of cis- and trans- isomers) for synthesis

Flash point	81 °C DIN 51758
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1,5 %(V)
Upper explosion limit	No information available.
Vapour pressure	ca.1 hPa at 50 °C
Relative vapour density	4,9
Density	ca.0,86 g/cm <sup>3</sup> at 60 °C
Relative density	No information available.
Water solubility	1,8 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 2,86 OECD Test Guideline 107 Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

## 9.2 Other data

Ignition temperature	375 °C DIN 51794
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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.  
The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### 10.2 Chemical stability

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

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No.	814442
Product name	3,3,5-Trimethylcyclohexanol (mixture of cis- and trans- isomers) for synthesis

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**10.3 Possibility of hazardous reactions**

Risk of ignition or formation of inflammable gases or vapours with:  
Oxidizing agents

**10.4 Conditions to avoid**

Strong heating.

**10.5 Incompatible materials**

no information available

**10.6 Hazardous decomposition products**

no information available

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**SECTION 11. Toxicological information**

**11.1 Information on toxicological effects**

*Acute oral toxicity*

LD50 Rat: 3.250 mg/kg (IUCLID)

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract., Nausea, Vomiting

*Acute inhalation toxicity*

Symptoms: Cough, Shortness of breath, mucosal irritations, Possible damages:, damage of respiratory tract

*Acute dermal toxicity*

LD50 Rabbit: 2.430 mg/kg (IUCLID)

*Skin irritation*

Rabbit

Result: slight irritation  
(RTECS)

*Eye irritation*

Rabbit

Result: Eye irritation  
(RTECS)

Causes serious eye irritation.

*Sensitisation*

Sensitisation test: Guinea pig

Result: negative

Method: OECD Test Guideline 406

*Germ cell mutagenicity*

*Genotoxicity in vitro*

Ames test

Result: negative  
(IUCLID)

*Carcinogenicity*

This information is not available.

*Reproductive toxicity*

This information is not available.

*Teratogenicity*

This information is not available.

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No.	814442
Product name	3,3,5-Trimethylcyclohexanol (mixture of cis- and trans- isomers) for synthesis

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*Specific target organ toxicity - single exposure*

May cause respiratory irritation.

*Specific target organ toxicity - repeated exposure*

This information is not available.

*Aspiration hazard*

This information is not available.

## 11.2 Further information

Systemic effects:

agitation, Diarrhoea, Dizziness, drowsiness

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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## SECTION 12. Ecological information

### 12.1 Toxicity

*Toxicity to fish*

LC50 Danio rerio (zebra fish): 50 mg/l; 96 h

OECD Test Guideline 203

*Toxicity to daphnia and other aquatic invertebrates*

EC50 Daphnia magna (Water flea): 96 mg/l; 24 h (IUCLID)

NOEC Daphnia magna (Water flea): 25 mg/l; 21 d

OECD Test Guideline 202

*Toxicity to algae*

IC50 Desmodesmus subspicatus (green algae): 25,8 mg/l; 72 h (IUCLID)

*Toxicity to bacteria*

EC10 Pseudomonas putida: 289 mg/l; 6 h (IUCLID)

### 12.2 Persistence and degradability

*Biodegradability*

1,5 %; 28 d

OECD Test Guideline 301D

Not readily biodegradable.

### 12.3 Bioaccumulative potential

*Partition coefficient: n-octanol/water*

log Pow: 2,86

OECD Test Guideline 107

Bioaccumulation is not expected.

### 12.4 Mobility in soil

No information available.

### 12.5 Results of PBT and vPvB assessment

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

Substance(s) in the mixture do(es) not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII, or a PBT/vPvB assessment was not conducted.

### 12.6 Other adverse effects

*Additional ecological information*

Discharge into the environment must be avoided.



SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No.	814442
Product name	3,3,5-Trimethylcyclohexanol (mixture of cis- and trans- isomers) for synthesis

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## SECTION 13. Disposal considerations

### *Waste treatment methods*

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

### Land transport (ADR/RID)

**14.1 - 14.6** Not classified as dangerous in the meaning of transport regulations.

### Inland waterway transport (ADN)

Not relevant

### Air transport (IATA)

**14.1 - 14.6** Not classified as dangerous in the meaning of transport regulations.

### Sea transport (IMDG)

**14.1 - 14.6** Not classified as dangerous in the meaning of transport regulations.

### 14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

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## SECTION 15. Regulatory information

### 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

#### *EU regulations*

Major Accident Hazard 96/82/EC

Legislation Directive 96/82/EC does not apply

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

Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC not regulated

Regulation (EC) No 689/2008 concerning the export and import of dangerous chemicals not regulated

Substances of very high concern (SVHC) This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of  $\geq 0.1\%$  (w/w).

#### *National legislation*

Storage class 10

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No.	814442
Product name	3,3,5-Trimethylcyclohexanol (mixture of cis- and trans- isomers) for synthesis

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## 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.

H319	Causes serious eye irritation.
H335	May cause respiratory irritation.

### Full text of R-phrases referred to under sections 2 and 3

R36/37	Irritating to eyes and respiratory system.
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### Training advice

Provide adequate information, instruction and training for operators.

### Labelling

*Hazard pictograms*



*Signal word*

Warning

*Hazard statements*


H319 Causes serious eye irritation.  
H335 May cause respiratory irritation.

*Precautionary statements*

Response

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

### Labelling (67/548/EEC or 1999/45/EC)

Symbol(s)	 Xi	Irritant
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R-phrases(s)	36/37	Irritating to eyes and respiratory system.
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S-phrases(s)	24	Avoid contact with skin.
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EC-No.	204-122-7
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#### Reduced labelling (≤125 ml)

Symbol(s)	 Xi	Irritant
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### Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at [www.wikipedia.org](http://www.wikipedia.org).

### Regional representation

This information is given on the authorised Safety Data Sheet for your country.

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No.	814442
Product name	3,3,5-Trimethylcyclohexanol (mixture of cis- and trans- isomers) for synthesis

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*The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.*