

**SAFETY DATA SHEET**

according to Regulation (EC) No. 1907/2006

Revision Date 07.02.2014

Version 4.4

**SECTION 1. Identification of the substance/mixture and of the company/undertaking****1.1 Product identifier**

Catalogue No.	818801
Product name	2,3-Butanediol (mixture of meso- D- and L-form) 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.	513-85-9

**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.merck-chemicals.com">www.merck-chemicals.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**

This substance is not classified as dangerous according to European Union legislation.

**2.2 Label elements****Labelling (REGULATION (EC) No 1272/2008)**

Not a hazardous substance or mixture according to Regulation (EC) No. 1272/2008.

**2.3 Other hazards**

None known.

**SECTION 3. Composition/information on ingredients****3.1 Substance**

Formula	CH <sub>3</sub> CH(OH)CH(OH)CH <sub>3</sub>	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> (Hill)
EC-No.	208-173-6	
Molar mass	90,12 g/mol	

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

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Remarks No disclosure requirement according to Regulation (EC) No. 1907/2006

**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.

After skin contact: wash off with plenty of water. Remove contaminated clothing.

After eye contact: rinse out with plenty of water.

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**

We have no description of any toxic symptoms.

**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, Carbon dioxide (CO<sub>2</sub>), Foam, 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.

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

Forms explosive mixtures with air on intense heating.

**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. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

**6.2 Environmental precautions**

Do not empty into drains.

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

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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 dry 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.

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

*Hand protection*

full contact:

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

splash contact:

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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)).

*Respiratory protection*

required when dusts/vapours/aerosols are generated.

Empfohlener Filtertyp: Filter P 1 (acc. to DIN 3181) for solid particles of inert substances

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 empty into drains.

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**SECTION 9. Physical and chemical properties**

**9.1 Information on basic physical and chemical properties**

Form	liquid
Colour	colourless
Odour	odourless
Odour Threshold	not applicable
pH	ca. 7 at 20 °C Aqueous solution
Melting point	18 - 20 °C
Boiling point/boiling range	180 - 182 °C at 1.013 hPa
Flash point	96 °C DIN 51758
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	3,1 %(V)
Upper explosion limit	11,4 %(V)

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Vapour pressure	< 1 hPa at 20 °C
Relative vapour density	3,1
Relative density	1,00 g/cm <sup>3</sup> at 20 °C
Water solubility	at 20 °C soluble
Partition coefficient: n-octanol/water	log Pow: -0,92 (experimental) (Lit.) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	44,68 mPa.s at 25 °C
Explosive properties	Not classified as explosive.
Oxidizing properties	none

#### 9.2 Other data

Ignition temperature 395 °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.

#### 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 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: > 5.000 mg/kg (External MSDS)

*Acute inhalation toxicity*

This information is not available.

*Acute dermal toxicity*

This information is not available.

*Skin irritation*

rabbit

Result: No irritation

(External MSDS)

*Eye irritation*

rabbit

Result: No eye irritation

(External MSDS)

*Sensitisation*

Sensitisation test (Magnusson and Kligman):

Result: negative

Method: OECD Test Guideline 406

*Germ cell mutagenicity*

*Genotoxicity in vitro*

Ames test

Result: negative

(External MSDS)

*Carcinogenicity*

This information is not available.

*Reproductive toxicity*

This information is not available.

*Teratogenicity*

This information is not available.

*Specific target organ toxicity - single exposure*

This information is not available.

*Specific target organ toxicity - repeated exposure*

This information is not available.

*Aspiration hazard*

This information is not available.

### 11.2 Further information

Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.

Handle in accordance with good industrial hygiene and safety practice.

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## SECTION 12. Ecological information

### 12.1 Toxicity

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*Toxicity to daphnia and other aquatic invertebrates*  
EC50 Daphnia magna (Water flea): > 100 mg/l; 48 h  
OECD Test Guideline 202

*Toxicity to bacteria*  
EC20 activated sludge: > 1.000 mg/l; 30 min  
OECD Test Guideline 209

#### 12.2 Persistence and degradability

*Biodegradability*  
90 - 100 %; 14 d  
OECD Test Guideline 301A  
Readily biodegradable.

#### 12.3 Bioaccumulative potential

*Partition coefficient: n-octanol/water*  
log Pow: -0,92  
(experimental)  
(Lit.) 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.

#### 12.6 Other adverse effects

Discharge into the environment must be avoided.

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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*

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Major Accident Hazard Legislation 96/82/EC  
Directive 96/82/EC does not apply

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

## 15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

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## SECTION 16. Other information

### Training advice

Provide adequate information, instruction and training for operators.

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

The product does not need to be labelled in accordance with EC directives or respective national laws.

### 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.

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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.*