

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 07.10.2013

Version 4.4

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

1.1 Product identifier

Catalogue No.	800906
Product name	Diethyl ethylmalonate 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.

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

Identified uses	Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal (www.merck-chemicals.com).
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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: prodsafe@merckgroup.com

1.4 Emergency telephone number	Please contact the regional company representation in your country.
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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	$\text{C}_2\text{H}_5\text{CH}(\text{COOC}_2\text{H}_5)_2$	$\text{C}_9\text{H}_{16}\text{O}_4$ (Hill)
CAS-No.	133-13-1	
EC-No.	205-093-3	
Molar mass	188,22 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.
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3.2 Mixture
not applicable

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.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water, Carbon dioxide (CO₂), 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.

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.

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapours, aerosols. 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

Cover drains. Collect, bind, and pump off spills.

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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.

6.4 Reference to other sections

Indications about waste treatment see section 13.

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.

Store at +15°C to +25°C.

7.3 Specific end use(s)

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

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

8.2 Exposure controls

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:	butyl-rubber
Glove thickness:	0,7 mm
Break through time:	> 480 min

splash contact:

Glove material:	natural latex
Glove thickness:	0,6 mm
Break through time:	> 30 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 898 Butoject® (full contact), KCL 706 Lapren® (splash contact).

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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).

Respiratory protection

Not required; except in case of aerosol formation.

Environmental exposure controls

Do not empty into drains.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	ether-like
Odour Threshold	No information available.
pH	No information available.
Melting point	0 °C
Boiling point/boiling range	204 - 206 °C at 1.013 hPa
Flash point	88 °C Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	No information available.
Relative vapour density	No information available.
Relative density	1,00 g/cm ³ at 20 °C
Water solubility	2,87 g/l at 20 °C

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Partition coefficient: n-octanol/water log Pow: 1,8
(calculated)
Bioaccumulation is not expected. (External MSDS)

Auto-ignition temperature No information available.

Decomposition temperature Distillable in an undecomposed state at normal pressure.

Viscosity, dynamic No information available.

Explosive properties Not classified as explosive.

Oxidizing properties none

9.2 Other data

none

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

heat-sensitive

10.3 Possibility of hazardous reactions

Violent reactions possible with:
Strong oxidizing agents, strong reducing agents, Bases, acids

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

no information available

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 rat: > 2.000 mg/kg
OECD Test Guideline 401

Acute inhalation toxicity

This information is not available.

Acute dermal toxicity

LD50 rat: > 2.000 mg/kg
OECD Test Guideline 402

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Skin irritation

rabbit

Result: No irritation

OECD Test Guideline 404

Eye irritation

rabbit

Result: No eye irritation

OECD Test Guideline 405

Sensitisation

Sensitisation test: guinea pig

Result: negative

Method: OECD Test Guideline 406

Germ cell mutagenicity

This information is not available.

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.

SECTION 12. Ecological information

12.1 Toxicity

No information available.

12.2 Persistence and degradability

No information available.

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 1,8

(calculated)

Bioaccumulation is not expected. (External MSDS)

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 for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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

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

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 above the respective regulatory limit (> 0.1 % (w/w) Regulation (EC) No 1907/2006 (REACH), Article 57).

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.

Regional representation

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

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.