SAFETY DATA SHEET according to Regulation (EC) No. 1907/2006 Revision Date 20.03.2019

Version 4.8

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

Catalogue No.	809622
Product name	Ethyl acetoacetate for synthesis
REACH Registration Number	01-2119457642-36-xxxx
CAS-No.	141-97-9

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.merckgroup.com).

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 Please contact the regional company representation in number your country.

SECTION 2. Hazards identification

2.1 Classification of the substance or mixture **REGULATION (EC) No 1272/2008** Not a hazardous substance or mixture according to Regulation (EC) No. 1272/2008.

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

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Formula EC-No. Molar mass	CH₃COCH₂COOC₂H₅ 205-516-1 130,14 g/mol	C6H10O3 (Hill)
Remarks	No disclosure requirement according to Regulation (EC) No. 1907/2006.	

3.2 Mixture

Not applicable

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. Remove contact lenses.

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

Dizziness, Nausea, Headache Drying-out effect resulting in rough and chapped skin.

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, Foam, Carbon dioxide (CO2), 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.



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Further information

Remove container from danger zone and cool with water. 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. Keep away from heat and sources of ignition. 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 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 and neutralising material (e.g. Chemizorb® H⁺, Merck Art. No. 101595). 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.

Advice on protection against fire and explosion Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

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.

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

8.2 Exposure controls

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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: Glove thickness: Break through time:	butyl-rubber 0,7 mm > 480 min
Glove material: Glove thickness:	Viton (R) 0,70 mm

splash contact:

Glove material:	Viton (R)
Glove thickness:	0,70 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 890 Vitoject® (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).

Other protective equipment

Flame retardant antistatic protective clothing.

Respiratory protection

Not required; except in case of aerosol formation.

Environmental exposure controls

Do not let product enter drains.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form

liquid

The life science business of Merck operates as MilliporeSigma in the US and Canada



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Colour	colourless
Odour	characteristic ester-like
Odour Threshold	No information available.
рН	4,0 at 110 g/l 20 °C
Melting point	-53,3 °C Method: OECD Test Guideline 102
Boiling point/boiling range	180,6 °C at 1.013 hPa Method: OECD Test Guideline 103
Flash point	73,5 °C at 1.013 hPa
	Method: ISO 2719
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1,0 %(V)
Upper explosion limit	54 %(V)
Vapour pressure	0,26 hPa at 20 °C Method: OECD Test Guideline 104
Relative vapour density	4,48
Density	1,03 g/cm3 at 20 °C Method: OECD Test Guideline 109
Relative density	No information available.
Water solubility	130,3 g/l at 20 °C Method: OECD Test Guideline 105
Partition coefficient: n- octanol/water	log Pow: 0,8 (20 °C) OECD Test Guideline 117 Bioaccumulation is not expected.



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Catalogue No. Product name	809622 Ethyl acetoacetate for synthesis
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	1,696 mPa.s at 20 °C Method: OECD Test Guideline 114
Explosive properties	Not classified as explosive.
Oxidizing properties	none
9.2 Other data	
Ignition temperature	350 °C

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, Strong acids, Strong bases

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: > 5.000 mg/kg OECD Test Guideline 401

Acute inhalation toxicity

Symptoms: Possible damages:, mucosal irritations

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Acute dermal toxicity LD50 Rat: > 2.000 mg/kg OECD Test Guideline 402

Skin irritation Rabbit Result: No skin irritation OECD Test Guideline 404

Eye irritation Rabbit Result: slight irritation OECD Test Guideline 405

Sensitisation

Freund's complete adjuvant test Guinea pig Result: Does not cause skin sensitisation. Method: OECD Test Guideline 406

Patch test: human Result: negative

(IUCLID)

Germ cell mutagenicity Genotoxicity in vitro In vitro mammalian cell gene mutation test Result: negative Method: OECD Test Guideline 476

Ames test Escherichia coli/Salmonella typhimurium Result: negative Method: OECD Test Guideline 471

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.

Repeated dose toxicity Rat male and female Oral 28 d daily NOAEL: 1.000 mg/kg OECD Test Guideline 407

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Subacute toxicity, No significant adverse effects were reported *Aspiration hazard* This information is not available.

11.2 Further information

After absorption: Headache, Dizziness, Nausea However, when the product is handled appropriately, hazardous effects are unlikely to occur. Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish semi-static test LC50 Danio rerio (zebra fish): > 100 mg/l; 96 h Analytical monitoring: yes OECD Test Guideline 203

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

Toxicity to algae static test ErC50 Desmodesmus subspicatus (green algae): > 100 mg/l; 72 h Analytical monitoring: yes OECD Test Guideline 201

Toxicity to bacteria static test EC50 activated sludge: > 3.000 mg/l; 24 h fermentation tube test

12.2 Persistence and degradability

Biodegradability 66 %; 28 d; aerobic OECD Test Guideline 301D Readily biodegradable

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water log Pow: 0,8 (20 °C) OECD Test Guideline 117

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

Additional ecological information Discharge into the environment must be avoided.



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Ethyl acetoacetate for synthesis

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 - 14.6Not 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

<i>EU regulations</i> Major Accident Hazard	SEVESO III
Legislation	Not applicable
Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work.

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

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

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Catalogue No. Product name	809622 Ethyl acetoac	etate for synthesis
Substances of very high c	oncern (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 ≥ 0.1 % (w/w).
<i>National legislation</i> Storage class	10 - 13	

15.2 Chemical safety assessment

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

SECTION 16. Other information

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Signal word Warning

Hazard statements H227 Combustible liquid.

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.

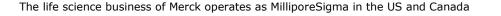
Regional representation

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.

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