

Chemical Safety Data Sheet MSDS / SDS

ETHYL ACETOACETATE (1,3-13C2)

Revision Date:2026-05-31 Revision Number:1

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

Product name : ETHYL ACETOACETATE (1,3-13C2)
CBnumber : CB5394254
CAS : 77504-73-5
Synonyms : Ethyl acetoacetate-1,3-13C?;Ethyl acetoacetate (1,3-13C?, 99%)

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

Precautionary statements

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

P302+P352 IF ON SKIN: wash with plenty of soap and water.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P271 Use only outdoors or in a well-ventilated area.

P264 Wash skin thoroughly after handling.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

Hazard statements

H315 Causes skin irritation

H319 Causes serious eye irritation

H335 May cause respiratory irritation

SECTION 3: Composition/information on ingredients

Substance

Product name	: ETHYL ACETOACETATE (1,3-13C2)
Synonyms	: Ethyl acetoacetate-1,3-13C?;Ethyl acetoacetate (1,3-13C?, 99%)
CAS	: 77504-73-5
MF	: C6H10O3
MW	: 132.16

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) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

4.4 Notes to physician

No data 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

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.

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 vapors, aerosols. Keep away from heat and sources of ignition. 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. Chemizorb®).

Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

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.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed.

Storage class

Storage class (TRGS 510): 10: Combustible liquids

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Change contaminated clothing. Wash hands after working with substance.

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

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 EN 16523-1 please contact the supplier of CE-

approved gloves (e.g. KCL GmbH, D-36124 Eichenzell,

Internet: www.kcl.de).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

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approved gloves (e.g. KCL GmbH, D-36124 Eichenzell,

Internet: www.kcl.de).

Splash contact

Material: Viton®

Minimum layer thickness: 0.7 mm

Break through time: 30 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Respiratory protection

Not required; except in case of aerosol formation.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

a) Physical state	liquid
b) Color	No data available

c) Odor	No data available
d) Melting point/freezing point	Melting point/range: -43 °C - lit.
e) Initial boiling point and boiling range	181 °C - lit.
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	84 °C - closed cup
i) Autoignition temperature	No data available
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	No data available
n) Partition coefficient n-octanol/water	No data available
o) Vapor pressure	No data available
p) Density	1.045 g/mL at 25 °C 1.045 g/cm ³ at 25 °C
Relative density	1.045 g/mL at 25 °C
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Chemical stability

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

10.2 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

Strong acids

Strong bases

10.3 Conditions to avoid

Strong heating.

10.4 Incompatible materials

No data available

10.5 Hazardous decomposition products

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - female - 10,800 mg/kg (OECD Test Guideline 401)

Remarks: The value is given in analogy to the following substances: ethyl acetoacetate

LC50 Inhalation - Rabbit - male and female - 4 h - > 49.2 mg/l - vapor

Remarks: (ECHA)

The value is given in analogy to the following substances: methyl acetate

Symptoms: Possible damages: mucosal irritations

LD50 Dermal - Rat - male and female - > 2,000 mg/kg (OECD Test Guideline 402)

Remarks: The value is given in analogy to the following substances: ethyl acetoacetate

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h (OECD Test Guideline 404)

Remarks: The value is given in analogy to the following substances: ethyl acetoacetate

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation - 24 h (OECD Test Guideline 405)

Remarks: The value is given in analogy to the following substances: ethyl acetoacetate

Respiratory or skin sensitization

Freund's complete adjuvant test - Guinea pig

Result: negative (OECD Test Guideline 406)

Remarks: The value is given in analogy to the following substances: ethyl acetoacetate

Germ cell mutagenicity

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster lung cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Remarks: The value is given in analogy to the following substances: ethyl acetoacetate

Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Remarks: The value is given in analogy to the following substances: ethyl acetoacetate

No data available

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 28 d - NOAEL (No observed adverse effect level) - 1,000 mg/kg

Remarks: Subacute toxicity

No significant adverse effects were reported

The value is given in analogy to the following substances: ethyl acetoacetate

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption:

Headache

Dizziness

Nausea

Other dangerous properties can not be excluded.

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 (OECD Test Guideline 203)

Remarks: The value is given in analogy to the following substances: ethyl acetoacetate

Toxicity to daphnia static test EC50 - Daphnia magna (Water flea) - > 100 mg/l - 48 h and other aquatic (OECD Test Guideline 202)

invertebrates Remarks: The value is given in analogy to the following substances: ethyl acetoacetate

Toxicity to algae static test ErC50 - Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h (OECD Test Guideline 201)

Remarks: The value is given in analogy to the following substances: ethyl acetoacetate

12.2 Persistence and degradability

Biodegradability aerobic Chemical oxygen demand - Exposure time 28 d

Result: 66 % - Readily biodegradable.

(OECD Test Guideline 301D)

Remarks: The value is given in analogy to the following substances: ethyl acetoacetate

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

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

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

14.1 UN number

ADR/RID: -

IMDG: -

IATA-DGR: -

14.2 UN proper shipping name

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA-DGR: Not dangerous goods

14.3 Transport hazard class(es)

ADR/RID: -

IMDG: -

IATA-DGR: -

14.4 Packaging group

ADR/RID: -

IMDG: -

IATA-DGR: -

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA-DGR: no

14.6 Special precautions for user

Based on chemical properties, choose appropriate tools and conditions of transport.

Transporting tools shall be equipped with appropriate and sufficient firefighting equipment and emergency leaking installations. If transporting by road, please go along the specified route.

14.7 Incompatible materials

SECTION 15: Regulatory information

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

National regulatory information

Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number : B1A222223531

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

Other regulations

Please pay attention on the waste treatment should also comply with local regulations requirement.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.