Chemical Safety Data Sheet MSDS / SDS

Ethyl 4,4,4-trifluoroacetoacetate

Revision Date:2025-07-26 Revision Number:1

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

Product identifier

Product name	: Ethyl 4,4,4-trifluoroacetoacetate					
CBnumber	: CB1133091					
CAS	: 372-31-6					
EINECS Number	: 206-750-7					
Synonyms	: ethyl 4,4,4-trifluoro-3-oxobutanoate,Ethyl 4,4,4-trifluoroacetoacetate					
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

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

P240 Ground/bond container and receiving equipment.

P241 Use explosion-proof electrical/ventilating/lighting/.../equipment.

P273 Avoid release to the environment.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

Hazard statements

H226 Flammable liquid and vapour

H302 Harmful if swallowed

H402 Harmful to aquatic life

H412 Harmful to aquatic life with long lasting effects

SECTION 3: Composition/information on ingredients

Substance

: Ethyl 4,4,4-trifluoroacetoacetate
: ethyl 4,4,4-trifluoro-3-oxobutanoate,Ethyl 4,4,4-trifluoroacetoacetate
: 372-31-6
: 206-750-7
: C6H7F3O3
: 184.11

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Dry powder Dry sand

Unsuitable extinguishing media

Do NOT use water jet.

Special hazards arising from the substance or mixture

Carbon oxides, Hydrogen fluoride

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

Use water spray to cool unopened containers.

NFPA 704

2	3	0
HEALTH	2	Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. <u>diethyl</u> <u>ether</u> , ammonium phosphate, iodine)
FIRE	3	Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature conditions . Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, <u>acetone</u>)
REACT	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, N2)
SPEC. HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas. For personal protection see section 8.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Store in cool place.

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

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	colorless clear, liquid
Odour	No data available
Odour Threshold	No data available
pH	6,2 at 10 g/l
Melting point/freezing point	Melting point/range: -39 °C
Initial boiling point and boiling range	129 - 130 °C - lit.
Flash point	38 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive	No data available
limits	
Vapour pressure	8 hPa at 20 °C
Vapour density	No data available
Relative density	1,259 g/cm3 at 25 °C
Water solubility	slightly soluble
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

Other safety information

No data available

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

Heat, flames and sparks.

Incompatible materials

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen fluoride Other decomposition products - No data available In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 855 mg/kg Skin corrosion/irritation Skin - Rabbit Result: Mild skin irritation - 4 h Serious eye damage/eye irritation No data available Respiratory or skin sensitization No data available Germ cell mutagenicity No data available Carcinogenicity IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC. **Reproductive toxicity** No data available Specific target organ toxicity - single exposure No data available Specific target organ toxicity - repeated exposure No data available Aspiration hazard No data available Additional Information **RTECS: Not available** To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

Toxicity

Toxicity to fish

LC50 - Oncorhynchus mykiss (rainbow trout) - > 101,0 mg/l - 96,0 h

Toxicity to daphnia and other aquatic

EC50 - Daphnia magna (Water flea) - 27 mg/l - 48 h

invertebrates

Persistence and degradability

Biodegradability Result: - Not readily biodegradable.

Bioaccumulative potential

No data available

Mobility in soil

No data available

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Other adverse effects

Harmful to aquatic life with long lasting effects. No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 3272 IMDG: 3272 IATA: 3272

UN proper shipping name

ADR/RID: ESTERS, N.O.S. (Ethyl 4,4,4-trifluoroacetoacetate) IMDG: ESTERS, N.O.S. (Ethyl 4,4,4-trifluoroacetoacetate) IATA:

Esters, n.o.s. (Ethyl 4,4,4-trifluoroacetoacetate) 14.3

Transport hazard class(es)

		IATA:
ADR/RID: 3 IMDG: 3		
Packaging group 14.4 ADR/RID: III IMDG: III		IATA:
ADR/RID: III IVIDG: III		III
	Chemical Book	

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ADR/RID: no IMDG Marine pollutant: no

Special precautions for user

No data available

SECTION 15: Regulatory information

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

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: https://www.mem.gov.cn/

Measures for Environmental Management of New Chemical Substances

EC Inventory:Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: https://echa.europa.eu/

New Zealand Inventory of Chemicals (NZIoC):Listed. website: https://www.epa.govt.nz/

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: https://emb.gov.ph/

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: https://www.epa.gov/

Vietnam National Chemical Inventory:Listed. website: https://chemicaldata.gov.vn/

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: https://www.mee.gov.cn/

Korea Existing Chemicals List (KECL):Not Listed. website: http://ncis.nier.go.kr

SECTION 16: Other information

Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road CAS: Chemical Abstracts Service EC50: Effective Concentration 50% IATA: International Air Transportation Association IMDG: International Maritime Dangerous Goods LC50: Lethal Concentration 50% LD50: Lethal Dose 50% RID: Regulation concerning the International Carriage of Dangerous Goods by Rail STEL: Short term exposure limit

TWA: Time Weighted Average

References

- [1] CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple
- [2] ChemlDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp
- [3] ECHA European Chemicals Agency, website: https://echa.europa.eu/
- [4] eChemPortal The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

[5] ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg Chemical Book

no

- [6] Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp
- [7] HSDB Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm
- [8] IARC International Agency for Research on Cancer, website: http://www.iarc.fr/
- [9] IPCS The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home
- [10] Sigma-Aldrich, website: https://www.sigmaaldrich.com/

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.