



Safety Data Sheet - Version 5.0

Preparation Date 9/15/2015

Latest Revision Date (If Revised)

1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1 Product Identifier

Chemical Name 4,4,4-Trifluoro-3-oxobutanoic Acid Ethyl Ester

Catalogue # T792060

1.2 Relevant Identified Uses of the Substance or Mixture and Uses Advised Against

Product Uses To be used only for scientific research and development. Not for use in humans or animals.

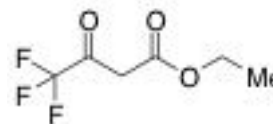
1.3 Details of the Supplier of the Safety Data Sheet

Company Toronto Research Chemicals
2 Brisbane Road
Toronto, ON M3J 2J8
CANADA

Telephone +14166659696

FAX +14166654439

Email orders.trc@lqcgroup.com



1.4 Emergency Telephone Number

Emergency# +1(416) 665-9696 between 0800-1700 (GMT-5)

2. HAZARDS IDENTIFICATION

2.1/2.2 Classification of the Substance or Mixture and Label Elements

GHS Hazards Classification (According to EU Regulation 1272/2008 and US OSHA 1910.1200)

Flammable Liquids (Category 3)

Acute Toxicity, Oral (Category 4)

Skin Irritation (Category 3)

Hazardous to the Aquatic Environment, Acute Hazard (Category 3)

Hazardous to the Aquatic Environment, Long-Term Hazard (Category 3)

GHS Hazards Identification (According to EU Regulation 1272/2008 and US OSHA 1910.1200)

Signal Word Warning



GHS Hazard Statements

H226 Flammable liquid and vapour.

H302 Harmful if swallowed.

H316 Causes mild skin irritation.

H402 Harmful to aquatic life.

H412 Harmful to aquatic life with long lasting effects.

GHS Precautionary Statements

P273 Avoid release to the environment.

2.3 Unclassified Hazards/Hazards Not Otherwise Classified

No data available.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Molecular Formula: C₅H₄F₃O₃

Molecular Weight: 184.11

Synonyms

4,4,4-Trifluoroacetoacetic Acid Ethyl Ester; 1-Ethoxy-4,4,4-trifluorobutane-1,3-dione; 4,4,4-Trifluoro-3-oxo-butyric Acid Ethyl Ester; 4,4,4-Trifluoro-3-oxobutanoic Acid Ethyl Ester; 4,4,4-Trifluoroacetoacetic Acid Ethyl Ester; Ethyl (Trifluoroacetyl)acetate; Ethyl 3-oxo-4,4,4-Trifluorobutanoate; Ethyl 4,4,4-Trifluoro-3-oxobutanoate; Ethyl 4,4,4-Trifluoro-3-oxobutyrate; Ethyl 4,4,4-Trifluoroacetoacetate; Ethyl 4,4,4-Trifluoroacetylacetate; Ethyl Trifluoroacetoacetate; Ethyl γ,γ,γ -Trifluoroacetoacetate; Ethyl ω,ω,ω -Trifluoroacetoacetate; NSC 42739; NSC 49750

3.2 Mixtures

Not a mixture.

4. FIRST AID MEASURES**4.1 Description of First Aid Measures****General Advice**

If medical attention is required, show this safety data sheet to the doctor.

If Inhaled

If inhaled, move person to fresh air. If not breathing, give artificial respiration and consult a physician.

In Case of Skin Contact

Wash affected area with soap and water. Consult a physician if any exposure symptoms are observed.

In Case of Eye Contact

Immediately rinse eyes with plenty of water for at least 15 minutes. Consult a physician.

If Swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Do NOT induce vomiting unless advised to do so by a physician or Poison Control Center. Seek medical attention.

4.2 Most Important Symptoms and Effects. Both Acute and Delayed

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

4.3 Indication of any Immediate Medical Attention and Special Treatment Needed

No data available.

5. FIREFIGHTING MEASURES**5.1 Extinguishing Media****Conditions of flammability**

Flammable in the presence of a source of ignition when the temperature is above the flash point. Keep away from heat/sparks/open flame/hot surface. No Smoking.

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special Hazards Arising from the Substance or Mixture

Carbon oxides, Hydrogen fluoride

5.3 Advice for Firefighters

Wear self contained breathing apparatus for fire fighting if necessary. Use personal protection equipment.

5.4 Further Information

No data available.

6. ACCIDENTAL RELEASE MEASURES**6.1 Personal Precautions, Protective Equipment and Emergency Procedures**

Use recommended personal protective equipment (see Section 8). Adequate ventilation must be provided to ensure vapours or mists are not inhaled. Vapours are heavier than air and may accumulate in low areas. All sources of ignition, including sources of static discharge, must be removed from area.

6.2 Environmental Precautions

Material should not be allowed to enter the environment. Prevent further spillage or discharge into drains, if safe to do so.

6.3 Methods and Materials for Containment and Cleaning Up

Contain the spill and then collect using non-combustible absorbent material (such as clay, diatomaceous earth, vermiculite or other appropriate material). Place material in a suitable, sealable container and then dispose according to local/national regulations and guidance (see Section 13).

6.4 Reference to Other Sections

For protective equipment, refer to Section 8. For disposal, see Section 13.

7. HANDLING AND STORAGE

7.1 Precautions for Safe Handling

Avoid contact with skin and eyes. Ventilation and proper handling are to be used to prevent the formation of vapours and mists. Remove all sources of ignition and take precautionary measures to prevent the buildup of electrostatic discharge (ground and bond containers as appropriate). No smoking, eating or drinking around this material. Wash hands after use.

7.2 Conditions for Safe Storage, Including any Incompatibilities

Ensure container is kept securely closed before and after use. Keep in a well ventilated area and do not store with strong oxidizers or other incompatible materials (see Section 10).

Storage conditions: 4°C

7.3 Specific End Uses

For scientific research and development only. Not for use in humans or animals.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control Parameters

Contains no components with established occupational exposure limits.

8.2 Exposure Controls

Appropriate Engineering Controls

A laboratory fumehood or other appropriate form of local exhaust ventilation should be used to avoid exposure.

Personal Protective Equipment

All recommendations below are advisory in nature and a risk assessment should be performed by the employer/end user prior to use of this product. The type of protective equipment must be selected based on the amount and concentration of the dangerous material being used in the workplace.

Eye/Face Protection

Safety glasses or safety goggles. All equipment should have been tested and approved under appropriate standards, such as NIOSH (US), CSA (Canada), or EN 166 (EU).

Skin Protection

Gloves should be used when handling this material. Gloves are to be inspected prior to use. Contaminated gloves are to be removed using proper glove removal technique so that the outer surface of the glove does not contact bare skin. Dispose of contaminated gloves after use in compliance with good laboratory practices and local requirements.

Gloves used for incidental exposures (splash protection) should be designated as "low chemical resistant" or "waterproof" by EU standard EN 374. Unrated gloves are not recommended.

Suggested gloves: AnsellPro nitrile gloves style 92-500 or 92-600, 5 mil thickness.

Penetration time has not been determined.

Gloves used for prolonged direct exposure (immersion) should be designated "chemical resistant" as per EN 734 with the resistance codes corresponding to the anticipated use of the material.

Suggested gloves: AnsellPro Viton/Butyl gloves style 38-612, 4/8 mil thickness.

Penetration time has not been determined.

These recommendations may not apply if the material is mixed with any other chemical, or dissolved into a solution. A risk assessment must be performed to ensure the gloves will still offer acceptable protection.

Body Protection

Fire resistant (Nomex) lab coat or coveralls.

Respiratory Protection

Recommended respirators are NIOSH-approved OV/Multi-Gas/P95 or CEN-approved ABEK-P2 respirators. These are to be only used as a backup to local exhaust ventilation or other engineering controls. If the respirator is the only means of protection, a full-face supplied air respirator must be used.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on Basic Physical and Chemical Properties

A) Appearance

Clear Colorless Oil

C) Odour Threshold

No data available.

E) Melting Point/Freezing Point

No Data Available

G) Flash point

38 °C (100 °F) - closed cup

I) Flammability (Solid/Gas)

No data available.

K) Vapour Pressure

8 hPa (6 mmHg) at 20 °C (68 °F)

M) Relative Density

1.259 g/cm³ at 25 °C (77 °F)

O) Partition Coefficient: n-octanol/water

No data available.

Q) Decomposition Temperature

No data available.

S) Explosive Properties

No data available.

B) Odour

No data available.

D) pH

No data available.

F) Initial Boiling Point/Boiling Range

No data available.

H) Evaporation Rate

No data available.

J) Upper/Lower Flammability/Explosive Limits

No data available.

L) Vapour Density

No data available.

N) Solubility

Chloroform, Methanol

P) Auto-Ignition Temperature

No data available.

R) Viscosity

No data available.

T) Oxidizing Properties

No data available.

9.2 Other Information

no data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available.

10.2 Chemical Stability

Stable under recommended storage conditions.

10.3 Possibility of Hazardous Reactions

No data available.

10.4 Conditions to Avoid

Heat, flames and sparks.

10.5 Incompatible Materials

Oxidizing agents, Strong acids, Strong bases, Strong reducing agents.

10.6 Hazardous Decomposition Products

Other decomposition products: No data available. In the event of fire: see section 5.

11. TOXICOLOGICAL INFORMATION

11.1 Information on Toxicological Effects

A) Acute Toxicity

Oral LD₅₀: Rat - 855 mg/kg

Dermal LD₅₀: No data available.

Inhalation LC₅₀: No data available.

B) Skin Corrosion/Irritation

Moderate skin irritant.

C) Serious Eye Damage/Irritation

No data available

D) Respiratory or Skin Sensitization

No data available

E) Germ Cell Mutagenicity

No data available

F) Carcinogenicity

No data available

G) Reproductive Toxicity/Teratogenicity

No data available

H) Single Target Organ Toxicity - Single Exposure

No data available

I) Single Target Organ Toxicity - Repeated Exposure

No data available

J) Aspiration Hazard

No data available

K) Potential Health Effects and Routes of Exposure

Inhalation

May be harmful if inhaled. May cause respiratory tract irritation.

Ingestion

Harmful if swallowed.

Skin

Harmful if absorbed through skin. May cause skin irritation.

Eyes

May cause eye irritation.

L) Signs and Symptoms of Exposure

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

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

M) Additional Information

RTECS: Not available.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish:

LC50 - Oncorhynchus mykiss (rainbow trout) - > 101.0 mg/l - 96.0 h

Toxicity to daphnia and other aquatic invertebrates:

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

12.2 Persistence and Degradability

Not readily biodegradable.

12.3 Bioaccumulative Potential

No data available.

12.4 Mobility in Soil

No data available.

12.5 Results of PBT and vPvB Assessment

No data available.

12.6 Other Adverse Effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Harmful to aquatic life with long lasting effects.

13. DISPOSAL CONSIDERATIONS

13.1 Waste Treatment Methods

A) Product

Product may be burned in an incinerator equipped with afterburner and scrubber. Excess and expired materials are to be offered to a licensed hazardous material disposal company. Ensure that all Federal and Local regulations regarding the disposal and destruction of this material are followed.

B) Contaminated Packaging

Dispose of as above.

C) Other Considerations

Product is not to be disposed of in sanitary sewers, storm sewers, or landfills.

14. TRANSPORT INFORMATION

14.1 UN Number

DOT (US): UN3272

IATA: UN3272

IMDG: UN3272

ADR/RID: UN3272

14.2 UN Proper Shipping Name

DOT (US)/IATA:

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

IMDG/ARD/RID:

ESTERS, N.O.S. (Ethyl 4,4,4-trifluoroacetoacetate)

14.3 Transport Hazard Class(es)

DOT (US): 3

IATA: 3

IMDG: 3

ADR/RID: 3

14.4 Packing Group

DOT (US): III

IATA: III

IMDG: III

ADR/RID: III

14.5 Environmental Hazards

DOT (US): None

IATA: None

IMDG: None

ADR/RID: None

14.6 Special Precautions for User

None

15. REGULATORY INFORMATION

This safety data sheet complies with the requirements of WHMIS (Canada), OSHA 1910.1200 (US), and EU Regulation EC No. 1907/2006 (European Union).

15.1 Safety, Health and Environmental Regulations/Legislation Specific for the Substance or Mixture**A) Canada**

DSL/NDSL Status: This product or a component of this product is registered on the Canadian DSL/NDSL.

B) United States

TSCA Status: This product or a component is listed on the US EPA TSCA.

C) European Union

ECHA Status: This product or a component is registered with the EU ECHA.

15.2 Chemical Safety Assessment

No data available

16. OTHER INFORMATION**16.1 Revision History**

Original Publication Date: 9/15/2015

16.2 List of Abbreviations

LD50	Median lethal dose of a substance required to kill 50% of a test population.
LC50	Medial lethal concentration of a substance required to kill 50% of a test population.
LDLo	Lowest known lethal dose
TDLo	Lowest known toxic dose
IARC	International Agency for Research on Cancer
NTP	National Toxicology Program
RTECS	Registry of Toxic Effects of Chemical Substances

16.3 Further Information

Copyright 2015. Toronto Research Chemicals Inc. Copies may be made for internal use only. The above information is believed to be correct to the best of our knowledge, but is to be only used as a guide. To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. Please take all due care when handling this product.