

Chemical Safety Data Sheet MSDS / SDS

METHYL 4,4,4-TRIFLUOROCROTONATE

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

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

Product name : METHYL 4,4,4-TRIFLUOROCROTONATE
CBnumber : CB3392074
CAS : 85694-31-1
Synonyms : (E)-methyl 4,4,4-trifluorobut-2-enoate,2-Butenoic acid, 4,4,4-trifluoro-, methyl ester

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.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P405 Store locked up.

Hazard statements

H226 Flammable liquid and vapour
H315 Causes skin irritation
H319 Causes serious eye irritation
H335 May cause respiratory irritation

SECTION 3: Composition/information on ingredients

Substance

Product name	: METHYL 4,4,4-TRIFLUOROCROTONATE
Synonyms	: (E)-methyl 4,4,4-trifluorobut-2-enoate, 2-Butenoic acid, 4,4,4-trifluoro-, methyl ester
CAS	: 85694-31-1
MF	: C ₅ H ₅ F ₃ O ₂
MW	: 154.09

SECTION 4: First aid measures

General Advice

If symptoms persist, call a physician.

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

Inhalation

Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.

Ingestion

Clean mouth with water and drink afterwards plenty of water.

Most important symptoms and effects

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

Self-Protection of the First Aider

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

Notes to Physician

Treat symptomatically.

SECTION 5: Firefighting measures

Suitable Extinguishing Media

Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

No information available.

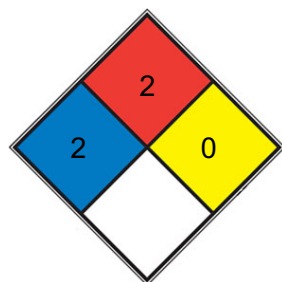
Specific Hazards Arising from the Chemical

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA 704



HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

FIRE 2 Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, [sulfur](#))

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

Ensure adequate ventilation. Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.

Environmental Precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: Handling and storage

Handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take precautionary measures against static discharges.

Storage

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat, sparks and flame.

Specific Use(s)

Use in laboratories

SECTION 8: Exposure controls/personal protection

Control Parameters

Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours MDHS 88

Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

Exposure Controls

Engineering Measures

Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

Personal protective equipment

Eye Protection

Goggles (European standard - EN 166)

Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers	-	EN 374	(minimum requirement)
Neoprene	recommendations			
Natural rubber				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.

(Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Skin and body protection

Long sleeved clothing

Respiratory Protection

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.

To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to EN14387

Small scale/Laboratory use

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

When RPE is used a face piece Fit Test should be conducted

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls

No information available.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Colorless

Physical State

Liquid

Odor

No information available

Odor Threshold

No data available

pH

No information available

Melting Point/Range

No data available

Softening Point

No data available

Boiling Point/Range

94 - 95 °C / 201.2 - 203 °F

Flash Point

No information available

Method - No information available

Evaporation Rate

No data available

Flammability (solid,gas)

Not applicable Liquid

Explosion Limits

No data available

Vapor Pressure

No data available

Vapor Density

No data available (Air = 1.0)

Specific Gravity / Density

1.237

Bulk Density

Not applicable Liquid

Water Solubility

Immiscible

Solubility in other solvents

No information available

Partition Coefficient (n-octanol/water)

No data available

Autoignition Temperature

No data available

Decomposition Temperature

No data available

Viscosity

No data available

Explosive Properties

explosive air/vapour mixtures possible

Oxidizing Properties

No information available

Molecular Formula

CF₃ CH=CHCO₂ CH₃

Molecular Weight

154.10

Colour

Clear

SECTION 10: Stability and reactivity**Stability**

Stable under normal conditions.

Hazardous Reactions

None under normal processing.

Hazardous Polymerization

No information available.

Conditions to Avoid

Keep away from open flames, hot surfaces and sources of ignition.

Materials to avoid

No information available.

Hazardous Decomposition Products

None under normal use conditions.

SECTION 11: Toxicological information**Product Information**

(a) acute toxicity;

(b) skin corrosion/irritation;

Category 2

(c) serious eye damage/irritation;

Category 2

(d) respiratory or skin sensitization;

	Respiratory		No data available									
	Skin		No data available									
(e)	germ cell mutagenicity;		No data available									
(f)	carcinogenicity;		No data available									
			There are no known carcinogenic chemicals in this product									
(g)	reproductive toxicity;		No data available									
(h)	STOT-single exposure;		Category 3									
	Results / Target organs		Respiratory system									
(i)	STOT-repeated exposure;		No data available									
	Target Organs		No information available.									
(j)	aspiratory hazard;		No data available									
Symptoms	/ effects, both acute and delayed		Symptoms of overexposure may be									

SECTION 12: Ecological information

Ecotoxicity effects

Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

Persistence and Degradability**Persistence**

Immiscible with water, Persistence is unlikely, based on information available.

Bioaccumulative Potential

May have some potential to bioaccumulate

Mobility in soil

Spillage unlikely to penetrate soil The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces Is not likely mobile in the environment due its low water solubility Will likely be mobile in the environment due to its volatility

Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

Persistent Organic Pollutant

This product does not contain any known or suspected substance

Ozone Depletion Potential

This product does not contain any known or suspected substance

SECTION 13: Disposal considerations

Waste from Residues/Unused Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging

Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

Other Information

Waste codes should be assigned by the user based on the application for which the product was used. Do not flush to sewer. Can be landfilled or incinerated, when in compliance with local regulations.

SECTION 14: Transport information

Road and Rail Transport

UN-No

UN3272

Proper Shipping Name

ESTERS, N.O.S.

Technical Shipping Name

(Methyl 4,4,4-trifluorocrotonate)

Hazard Class

3

Packing Group

III

IMDG/IMO

UN-No

UN3272

Proper Shipping Name

ESTERS, N.O.S.

Technical Shipping Name

(Methyl 4,4,4-trifluorocrotonate)

Hazard Class

3

Packing Group

III

IATA

UN-No

UN3272

Proper Shipping Name

ESTERS, N.O.S.*

Technical Shipping Name

(Methyl 4,4,4-trifluorocrotonate)

Hazard Class

3

Packing Group

III

Special Precautions for User

No special precautions required

SECTION 15: Regulatory information

International Inventories

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

National Regulations

SECTION 16: Other information

Prepared By

Health, Safety and Environmental Department

Revision Date

24-Oct-2025

Revision Summary

Not applicable.

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene. Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Legend

CAS

Chemical Abstracts Service

TSCA

United States Toxic Substances Control Act Section 8(b)

Inventory

EINECS/ELINCS

European Inventory of Existing Commercial Chemical

Substances/EU List of Notified Chemical Substances

DSL/NDSL

Canadian Domestic Substances List/Non-Domestic

Substances List

PICCS

Philippines Inventory of Chemicals and Chemical Substances

ENCS

Japanese Existing and New Chemical Substances

IECSC

Chinese Inventory of Existing Chemical Substances

AICS

Australian Inventory of Chemical Substances

KECL

Korean Existing and Evaluated Chemical Substances

NZIoC

New Zealand Inventory of Chemicals

WEL

Workplace Exposure Limit

TWA

Time Weighted Average

ACGIH

American Conference of Governmental Industrial Hygienists

IARC

International Agency for Research on Cancer

DNEL

Derived No Effect Level

PNEC

Predicted No Effect Concentration

RPE

Respiratory Protective Equipment

LD50

Lethal Dose 50%

LC50

Lethal Concentration 50%

EC50

Effective Concentration 50%

NOEC

No Observed Effect Concentration

POW

Partition coefficient Octanol:Water

PBT

Persistent, Bioaccumulative, Toxic

vPvB

very Persistent, very Bioaccumulative

ICAO/IATA

International Civil Aviation Organization/International Air
Transport Association

IMO/IMDG

International Maritime Organization/International Maritime
Dangerous Goods Code

ADR

European Agreement Concerning the International Carriage of
Dangerous Goods by Road

MARPOL

International Convention for the Prevention of Pollution from
Ships

OECD

Organisation for Economic Co-operation and Development

ATE

Acute Toxicity Estimate

BCF

Bioconcentration factor

VOC

(Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Disclaimer

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