

Chemical Safety Data Sheet MSDS / SDS

Methyl 3-(trifluoromethyl)benzoate

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 3-(trifluoromethyl)benzoate
CBnumber : CB5733730
CAS : 2557-13-3
EINECS Number : 457-830-5
Synonyms : trifluoromethyl benzoate,methyl 3-(trifluoromethyl)benzoate

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

P405 Store locked up.

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

Continuerinsing.

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

Hazard statements

H335 May cause respiratory irritation

H319 Causes serious eye irritation

H315 Causes skin irritation

H226 Flammable liquid and vapour

H227 Combustible liquid

SECTION 3: Composition/information on ingredients

Substance

| | |
|--------------|---|
| Product name | : Methyl 3-(trifluoromethyl)benzoate |
| Synonyms | : trifluoromethyl benzoate,methyl 3-(trifluoromethyl)benzoate |
| CAS | : 2557-13-3 |
| EC number | : 457-830-5 |
| MF | : C9H7F3O2 |
| MW | : 204.15 |

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.

| | Methyl | 3-(trifluoromethyl)benzoate |
|--|--------|-----------------------------|
| Most important symptoms and effects | | |
| None reasonably foreseeable. 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 spray. Carbon dioxide (CO₂). Dry chemical. Chemical foam. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

No information available.

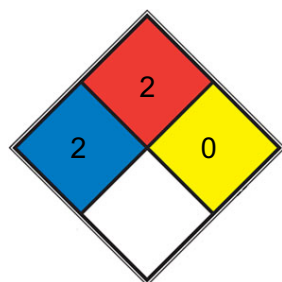
Specific Hazards Arising from the Chemical

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

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.

Methods for Containment and Clean Up

Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. Remove all sources of ignition.

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.

Storage

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

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 adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment. Ensure that eyewash stations and safety showers are close to the workstation location. 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 |
|----------------|-------------------|-----------------|-------------|-----------------------|
| Natural rubber | See manufacturers | - | EN 374 | (minimum requirement) |
| Butyl rubber | recommendations | | | |
| Nitrile rubber | | | | |
| Neoprene | | | | |
| 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

No protective equipment is needed under normal use conditions.

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

Small scale/Laboratory use

Maintain adequate ventilation

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

Light yellow

Physical State

Liquid

Odor

No information available

Odor Threshold

No data available

pH

No information available

Melting Point/Range

4 °C / 39.2 °

F Predicted data (ACD/Labs' ACD/PhysChem Suite)

Softening Point

No data available

Boiling Point/Range

211 - 214 °C / 411.8 - 417.2 °F @ 760 mmHg

Flash Point

84 °C / 183.2 °F Method - Based on available literature

Evaporation Rate

No data available

Flammability (solid,gas)

Not applicable Liquid

Explosion Limits

No data available

Vapor Pressure

0.002-0.023Pa at 20-50°C

Vapor Density

7.0 4 (Air = 1.0)

Specific Gravity / Density

1.290

Bulk Density

Not applicable Liquid

Water Solubility

Slightly soluble

Solubility in other solvents

No information available

Partition Coefficient (n-octanol/water)

No data available

desc_info

Component: Methyl 3-(trifluoromethyl)benzoate log Pow: 2.8

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

C9 H7 F3 O2

Molecular Weight

204.15

Colour

Colorless to Almost colorless

SECTION 10: Stability and reactivity

Stability

Stable under normal conditions.

Hazardous Reactions

None under normal processing.

Hazardous Polymerization

Hazardous polymerization does not occur.

Conditions to Avoid

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

Materials to avoid

Strong oxidizing agents.

Hazardous Decomposition Products

Carbon monoxide (CO). Carbon dioxide (CO₂). Gaseous hydrogen fluoride (HF). Fluorine.

SECTION 11: Toxicological information

Product Information

No acute toxicity information is available for this product

(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) aspiration hazard;

No data available

Other Adverse Effects

The toxicological properties have not been fully investigated.

Symptoms / effects,both acute and delayed

Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

SECTION 12: Ecological information

Ecotoxicity effects

Do not empty into drains.

| Component | Freshwater Fish | Water Flea | Freshwater Algae | Microtox |
|-----------|-----------------|------------|------------------|----------|
|-----------|-----------------|------------|------------------|----------|

| | | | | |
|------------------------------------|--|--|--|--|
| Methyl 3-(trifluoromethyl)benzoate | LC50: = 5.1 mg/L, 96h static (Danio rerio) | | | |
|------------------------------------|--|--|--|--|

Persistence and Degradability

Persistence

based on information available, May persist.

Bioaccumulative Potential

May have some potential to bioaccumulate

| Component | log Pow | Bioconcentration factor (BCF) |
|------------------------------------|---------|-------------------------------|
| Methyl 3-(trifluoromethyl)benzoate | 2.8 | No data available |

Mobility in soil

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

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. Do not empty into drains.

SECTION 14: Transport information

Road and Rail Transport

IMDG/IMO

Not regulated

IATA

Not regulated

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).

| Component | The Inventory of Hazardous Chemicals (2015 Edition) | List of dangerous goods GB 12268 - 2012 | TCSI | IECSC | EINECS | TSCA | DSL | PICCS | ENCS | ISHL | AICS | KECL |
|------------------------------------|---|---|------|-------|--------|------|-----|-------|------|------|------|------|
| | | | | | | | | | | | | |
| Methyl 3-(trifluoromethyl)benzoate | - | - | X | X | - | X | - | - | - | - | - | - |

National Regulations

SECTION 16: Other information

Prepared By

Health, Safety and Environmental Department

Revision Date

30-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

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

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.