

## Chemical Safety Data Sheet MSDS / SDS

## Trifluorothymine

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

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

## Product identifier

Product name : Trifluorothymine  
CBnumber : CB8684875  
CAS : 54-20-6  
EINECS Number : 200-197-5  
Synonyms : 5-(Trifluoromethyl)uracil,Trifluorothymine

## 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

Danger

## 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.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

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

H301 Toxic if swallowed

## SECTION 3: Composition/information on ingredients

### Substance

Product name	: Trifluorothymine
Synonyms	: 5-(Trifluoromethyl)uracil, Trifluorothymine
CAS	: 54-20-6
EC number	: 200-197-5
MF	: C <sub>5</sub> H <sub>3</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
MW	: 180.08

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## SECTION 4: First aid measures

### Description of first aid measures

#### General advice

Consult a physician. Show this 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. Take victim immediately to hospital. Consult a physician.

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### If swallowed

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

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## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing media

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

### Special hazards arising from the substance or mixture

Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), Hydrogen fluoride Combustible.

### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

## Further information

No data available

## NFPA 704



**HEALTH 0** Poses no health hazard, no precautions necessary and would offer no hazard beyond that of ordinary combustible materials

**FIRE 0** Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand. Materials that will not burn in air when exposed to a temperature of 820 °C (1,500 °F) for a period of 5 minutes.(e.g. Carbon tetrachloride)

**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

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

For personal protection see section 8.

### Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

### Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

### 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 formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

## Conditions for safe storage, including any incompatibilities

Store in cool place. Keep container tightly closed in a dry and well-ventilated place.

## Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## 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

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

#### 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, 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 particle respirator type N99 (US) or type P2 (EN 143) 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.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	white powder
Odour	No data available
Odour Threshold	No data available
pH	No data available

Melting point/freezing point	Melting point/range: 245 - 246 °C - lit.
Initial boiling point and boiling range	No data available
Flash point	No data available
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available
Relative density	No data available
Water solubility	methanol: soluble 50 mg/mL, clear
Partition coefficient: n-octanol/water	log Pow: 1,547
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

No data available

#### Incompatible materials

Strong oxidizing agents

#### Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), 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

No data available

LD50 Intraperitoneal - Mouse - 800 mg/kg

### Skin corrosion/irritation

No data available

### Serious eye damage/eye irritation

No data available

### Respiratory or skin sensitisation

No data available

### Germ cell mutagenicity Carcinogenicity

IARC: No component 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

#### Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation.

#### Specific target organ toxicity - repeated exposure

No data available

### Aspiration hazard

No data available

### Additional Information

RTECS: YR1750000

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

### Toxicity

LD50 intraperitoneal in mouse: 800mg/kg

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## SECTION 12: Ecological information

### Toxicity

No data available

### Persistence and degradability

No data available

### 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**

No data available

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## **SECTION 13: Disposal considerations**

#### **Waste treatment methods**

##### **Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

##### **Contaminated packaging**

Dispose of as unused product.

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## **SECTION 14: Transport information**

#### **UN number**

ADR/RID: 2811 IMDG: 2811 IATA: 2811

#### **UN proper shipping name**

ADR/RID: TOXIC SOLID, ORGANIC, N.O.S. (5-(Trifluoromethyl)uracil) IMDG: TOXIC SOLID, ORGANIC, N.O.S. (5-(Trifluoromethyl)uracil) IATA: Toxic solid, organic, n.o.s. (5-(Trifluoromethyl)uracil)

#### **Transport hazard class(es)**

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

#### **Packaging group**

ADR/RID: III IMDG: III IATA: III

#### **Environmental hazards**

ADR/RID: no IMDG Marine pollutant: no IATA: no

#### **Special precautions for user**

No data available

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## **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

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: <https://www.epa.gov/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: <https://emb.gov.ph/>

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: <https://www.epa.govt.nz/>

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

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

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

EC Inventory:Listed.

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

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## 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】 ChemIDplus, 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](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>

【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.