

Chemical Safety Data Sheet MSDS / SDS

S-(Trifluoromethyl)dibenzothiophenium tetrafluoroborateRevision Date:2025-02-01 Revision Number:1

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

Product name : S-(Trifluoromethyl)dibenzothiophenium tetrafluoroborate
CBnumber : CB9206124
CAS : 131880-16-5
Synonyms : Umemoto's reagent,5-(trifluoromethyl)-5H-dibenzo[b,d]thiophen-5-ium tetrafluoroborate

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 : 400-158-6606

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements****Pictogram(s)**

□

Signal word : Warning

Hazard statement(s)

H335 May cause respiratory irritation

H319 Causes serious eye irritation

H315 Causes skin irritation

Prevention

P271 Use only outdoors or in a well-ventilated area.

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

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P264 Wash ... thoroughly after handling.

Response

P319 Get medical help if you feel unwell.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

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

P362+P364 Take off contaminated clothing and wash it before reuse.

P332+P317 If skin irritation occurs: Get medical help.

P321 Specific treatment (see ... on this label).

P302+P352 IF ON SKIN: Wash with plenty of water/...

Storage

P405 Store locked up.

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

SECTION 3: Composition/information on ingredients

Substance

Product name	: S-(Trifluoromethyl)dibenzothiophenium tetrafluoroborate
Synonyms	: Umemoto's reagent,5-(trifluoromethyl)-5H-dibenzo[b,d]thiophen-5-ium tetrafluoroborate
CAS	: 131880-16-5
MF	: C13H8BF7S
MW	: 340.07

SECTION 4: First aid measures

Description of first aid measures

General advice

Hydrofluoric (HF) acid burns require immediate and specialized first aid and medical treatment. Symptoms may be delayed up to 24 hours depending on the concentration of HF. After decontamination with water, further damage can occur due to penetration/absorption of the fluoride ion. Treatment should be directed toward binding the fluoride ion as well as the effects of exposure. Skin exposures can be treated with a 2.5% calcium gluconate gel repeated until burning ceases. More serious skin exposures may require subcutaneous calcium gluconate except for digital areas unless the physician is experienced in this technique, due to the potential for tissue injury from increased pressure. Absorption can readily occur through the subungual areas and should be considered when undergoing decontamination. Prevention of absorption of the fluoride ion in cases of ingestion can be obtained by giving milk, chewable calcium carbonate tablets or Milk of Magnesia to conscious victims. Conditions such as hypocalcemia, hypomagnesemia and cardiac arrhythmias should be monitored for, since they can occur after exposure.

If inhaled

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

In case of skin contact

Wash off with soap and plenty of water. First treatment with calcium gluconate paste.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water.

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

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

Special hazards arising from the substance or mixture

Carbon oxides, Sulphur oxides, Hydrogen fluoride, Borane/boron oxides

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing vapours, mist or gas. For personal protection see section 8.

Environmental precautions

Do not let product enter drains.

Methods and materials for containment and cleaning up

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

Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

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

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

General industrial hygiene practice.

Personal protective equipment

Eye/face protection

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 EU Directive 89/686/EEC and the standard EN 374 derived from it.

Body Protection

Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Respiratory protection is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	solid
Odour	No data available
Odour Threshold	No data available

pH	No data available
Melting point/freezing point	Melting point/range: 162 - 164 °C
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	No data 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	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, Alkali metals, Amines

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Sulphur oxides, Hydrogen fluoride, Borane/boron oxides

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

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

No data available

Germ cell mutagenicity

No data available

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

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

Fluoride ion can reduce serum calcium levels possibly causing fatal hypocalcemia.

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

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

Other adverse effects

No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: - IMDG: - IATA: -

UN proper shipping name

ADR/RID: Not dangerous goods IMDG: Not dangerous goods IATA: Not dangerous goods

Transport hazard class(es)

ADR/RID: - IMDG: - IATA: -

Packaging group

ADR/RID: - IMDG: - IATA: -

Environmental hazards

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

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

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

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

Vietnam National Chemical Inventory:Not Listed. website: <https://chemicaldata.gov.vn/>

EC Inventory:Not Listed.

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

European Inventory of Existing Commercial Chemical Substances (EINECS):Not Listed. website: <https://echa.europa.eu/>

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

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

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

【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.