

Chemical Safety Data Sheet MSDS / SDS

1,1,1-TRIFLUORO-3-IODOBUTANERevision Date:2026-05-31 Revision Number:1

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

Product name : 1,1,1-TRIFLUORO-3-IODOBUTANE
CBnumber : CB9419575
CAS : 540-87-4
Synonyms : 1,1,1-trifluoro-3-iodobutane,3-iodo-1,1,1-trifluorobutane

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

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	: 1,1,1-TRIFLUORO-3-IODOBUTANE
Synonyms	: 1,1,1-trifluoro-3-iodobutane,3-Iodo-1,1,1-trifluorobutane
CAS	: 540-87-4
MF	: C4H6F3I
MW	: 237.99

SECTION 4: First aid measures

First Aid Measures

General advice

Immediate medical attention is required. In case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible). If symptoms persist, call a physician.

Eye contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. If symptoms persist, call a physician. Immediately flush with plenty of water. After initial flushing, remove any contact lenses and continue flushing for at least 15 minutes. Keep eye wide open while rinsing.

Skin Contact

Wash off immediately with plenty of water. Wash contaminated clothing before reuse. If skin irritation persists, call a physician. Immediate medical attention is not required. Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes.

Inhalation

Remove to fresh air. If symptoms persist, call a physician. Artificial respiration and/or oxygen may be necessary. Call a physician. Immediate medical attention is not required. Move to fresh air in case of accidental inhalation of vapors.

Ingestion

Immediate medical attention is not required. Rinse mouth. Drink plenty of water. Do NOT induce vomiting. Clean mouth with water and drink afterwards plenty of water. Never give anything by mouth to an unconscious person. Call a physician.

Self-protection of the first aider

Remove all sources of ignition. Use personal protective equipment as required.

Most important symptoms and effects, both acute and delayed

Symptoms

No information available.

Indication of any immediate medical attention and special treatment needed

Note to physicians

Treat symptomatically.

SECTION 5: Firefighting measures

Suitable Extinguishing Media

Suitable Extinguishing Media

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

Unsuitable Extinguishing Media

None.

Specific hazards arising from the chemical

Specific hazards arising from the chemical

Thermal decomposition can lead to release of toxic/corrosive gases and vapors.

Hazardous combustion products

Hydrogen fluoride. Carbon oxides. Phosgene.

Explosion data

Sensitivity to Mechanical Impact

No information available.

Sensitivity to Static Discharge

No information available.

Protective equipment and precautions for firefighters

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.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal precautions

Remove all sources of ignition. Evacuate personnel to safe areas. Ensure adequate ventilation, especially in confined areas. Use personal protective equipment as required.

Keep people away from and upwind of spill/leak.

Environmental precautions

Environmental precautions

Prevent further leakage or spillage if safe to do so. Prevent product from entering drains. Do not flush into surface water or sanitary sewer system. See Section 12 for additional

Ecological Information.

Methods and material for containment and cleaning up

Methods for containment

Prevent further leakage or spillage if safe to do so.

Methods for cleaning up

Pick up and transfer to properly labeled containers. Dam up. Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Soak up with inert absorbent material.

SECTION 7: Handling and storage

Precautions for safe handling

Advice on safe handling

Ensure adequate ventilation, especially in confined areas. Keep away from heat, sparks, flame and other sources of ignition (i.e., pilot lights, electric motors and static electricity).

Take precautionary measures against static discharges. Use spark-proof tools and explosion-proof equipment. All equipment used when handling the product must be grounded. Use with local exhaust ventilation. Use personal protective equipment as required. Do not breathe dust/fume/gas/mist/vapors/spray. Thermal decomposition can lead to release of toxic/corrosive gases and vapors.

Conditions for safe storage, including any incompatibilities

Storage Conditions

Keep tightly closed in a dry and cool place. Keep in properly labeled containers. Keep containers tightly closed in a cool, well-ventilated place. Store at 4 °C.

Incompatible materials

None known based on information supplied.

SECTION 8: Exposure controls/personal protection

Control parameters

Exposure Guidelines

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

Appropriate engineering controls

Engineering Controls

Showers

Eyewash stations

Ventilation systems

Individual protection measures, such as personal protective equipment

Eye/face protection

Tight sealing safety goggles. Face protection shield.

Skin and Body Protection

Wear protective gloves and protective clothing.

Respiratory protection

If exposure limits are exceeded or irritation is experienced, NIOSH/MSHA approved respiratory protection should be worn. Positive-pressure supplied air respirators may be required for high airborne contaminant concentrations. Respiratory protection must be provided in accordance with current local regulations.

General Hygiene Considerations

When using do not eat, drink or smoke. Regular cleaning of equipment, work area and clothing is recommended.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical State	liquid
Appearance	No information available
Odor	No information available
pH	No information available
Melting point/freezing point	-71.53 °C
Boiling point	103.5 °C
Flash point	34.55 °C
Density	1.83 g/mL
Evaporation rate	No information available
Upper flammability limits	No information available
Lower flammability limit	No information available
Vapor pressure	31.70
Vapor density	No information available
Specific gravity	No information available
Water solubility	No information available
Solubility in other solvents	No information available
Partition coefficient	3.41
Autoignition temperature	No information available
Decomposition temperature	No information available
Kinematic viscosity	No information available
Explosive properties	No information available
Oxidizing properties	No information available
Colour	Clear

SECTION 10: Stability and reactivity

Reactivity

Not applicable

Chemical stability

Stable under recommended storage conditions.

Possibility of Hazardous Reactions

None under normal processing.

Hazardous polymerization

No information available.

Conditions to avoid

Heat, flames and sparks.

Incompatible materials

Strong oxidizing agents.

Hazardous Decomposition Products

Hydrogen fluoride. Carbon oxides. Phosgene.

SECTION 11: Toxicological information

Information on likely routes of exposure

Inhalation

Classified based on available data. For more details, see section 2.

Eye contact

Classified based on available data. For more details, see section 2.

Skin Contact

Classified based on available data. For more details, see section 2.

Ingestion

Classified based on available data. For more details, see section 2.

Information on toxicological effects

Symptoms

Classified based on available data. For more details, see section 2.

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Chronic Toxicity

Avoid repeated exposure.

Numerical measures of toxicity - Product Information

Unknown acute toxicity

Classified based on available data. For more details, see section 2

SECTION 12: Ecological information

Ecotoxicity

May cause long lasting harmful effects to aquatic life

100% of the mixture consists of components(s) of unknown hazards to the aquatic environment.

Persistence and degradability

No information available.

Bioaccumulation

No information available.

Mobility

No information available.

SECTION 13: Disposal considerations

Disposal of wastes

Disposal should be in accordance with applicable regional, national and local laws and regulations.

Contaminated packaging

Do not reuse container.

Other Information

Waste codes should be assigned by the user based on the application for which the product was used.

SECTION 14: Transport information

DOT

UN/ID no

UN1993

Hazard Class

3

Packing Group

III

Proper shipping name

Flammable liquids, n.o.s.

Description

UN1993, Flammable liquids, n.o.s. (3-Iodo-1,1,1-trifluorobutane), 3, III

Emergency Response Guide Number

128

IMDG

UN/ID no

UN1993

Hazard Class

3

Packing Group

III

Proper shipping name

Flammable liquid, n.o.s.

Description

UN1993, Flammable liquid, n.o.s. (3-Iodo-1,1,1-trifluorobutane), 3, III, (34.55°C c.c.)

Special Provisions

223, 274, 955

EmS-No

F-E, S-E

IATA

UN/ID no

UN1993

Hazard Class

3

Packing Group

III

Proper shipping name

Flammable liquid, n.o.s.

Description

UN1993, Flammable liquid, n.o.s. (3-Iodo-1,1,1-trifluorobutane), 3, III

SECTION 15: Regulatory information

International Inventories

All of the components in the product are on the following Inventory lists

X - Listed

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

EINECS/ELINCS - European Inventory of Existing Chemical Substances/European List of Notified Chemical Substances

ENCS - Japan Existing and New Chemical Substances

IECSC - China Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

US Federal Regulations

SARA 313

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372.

SARA 311/312 Hazard Categories

Acute health hazard

Yes

Chronic Health Hazard

No

Fire hazard

Yes

Sudden release of pressure hazard

No

Reactive hazard

No

CWA (Clean Water Act)

This product does not contain any substances regulated as pollutants pursuant to the Clean Water Act (40 CFR 122.21 and 40 CFR 122.42).

US State Regulations

California Proposition 65

This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations

This product does not contain any substances regulated by state right-to-know regulations

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

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

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

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.