SAFETY DATA SHEETS

According to the UN GHS revision 9

Version: 1.0
Creation Date: July 15, 2019
Revision Date: July 15, 2019

SECTION 1: Identification

1.1 GHS Product identifier

Product name 4-chloro-α,α,α-trifluorotoluene

1.2 Other means of identification

Product number -
Other names Benzene, 1-chloro-4-(trifluoromethyl)-; p-Chlorbenzotrifluorid; 4-chloro-trifluoromethylbenzene

1.3 Recommended use of the chemical and restrictions on use

Identified uses Industrial and scientific research use.
Uses advised against no data available

1.4 Supplier's details

Company Shanghai Baishun Biotechnology Co., Ltd
Address No. 26, Lane 918, Lianye Road, Zhelin Town, Fengxian District, Shanghai, 201400, China
Telephone +86-21-37581181

1.5 Emergency phone number

Emergency phone number +86-21-37581181
Service hours Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

SECTION 2: Hazard identification

2.1 Classification of the substance or mixture

Flammable liquids, Category 3
Skin sensitization, Sub-category 1B
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 2

2.2 GHS label elements, including precautionary statements

Pictogram(s)

Signal word Warning
Hazard statement(s) H226 Flammable liquid and vapour
H317 May cause an allergic skin reaction
H411 Toxic to aquatic life with long lasting effects

Precautionary statement(s)
Prevention P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 Keep container tightly closed.
P240 Ground and bond container and receiving equipment.

	P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment. P242 Use non-sparking tools. P243 Take action to prevent static discharges. P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/... P261 Avoid breathing dust/fume/gas/mist/vapours/spray. P272 Contaminated work clothing should not be allowed out of the workplace. P273 Avoid release to the environment.
Response	P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower]. P370+P378 In case of fire: Use ... to extinguish. P302+P352 IF ON SKIN: Wash with plenty of water/... P333+P317 If skin irritation or rash occurs: Get medical help. P321 Specific treatment (see ... on this label). P362+P364 Take off contaminated clothing and wash it before reuse. P391 Collect spillage.
Storage	P403+P235 Store in a well-ventilated place. Keep cool.
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.

2.3 Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
4-chloro-α,α,α-trifluorotoluene	4-chloro-α,α,α-trifluorotoluene	98-56-6	202-681-1	100%

SECTION 4: First-aid measures

4.1 Description of necessary first-aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

4.2 Most important symptoms/effects, acute and delayed

SYMPTOMS: Symptoms of exposure to this compound include local irritation to skin, eyes and respiratory system, central nervous system depression and dermatitis due to defatting of the skin. Other symptoms include coughing, wheezing, a burning sensation, laryngitis, shortness of breath, headache, nausea, vomiting, lung irritation, chest pain, edema (which may be fatal), and irritation to mucous membranes. ACUTE/CHRONIC HAZARDS: This compound is an irritant of the skin, eyes and respiratory system. It is also extremely destructive to tissue of the mucous membranes. It is harmful if swallowed, inhaled or absorbed through the skin. High vapor concentrations cause anesthesia. When heated to decomposition it emits toxic fumes of hydrogen fluoride, hydrogen chloride and possibly organic fluorides. It also emits toxic fumes of carbon dioxide and carbon monoxide. (NTP, 1992)

4.3 Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Poisons A and B

SECTION 5: Fire-fighting measures

5.1 Suitable extinguishing media

Use dry chemical, carbon dioxide, or foam extinguishers. Vapors are heavier than air and will collect in low areas. Vapors may travel long distances to ignition sources and flashback. Vapors in confined areas may explode when exposed to fire. Containers may explode in fire. Storage containers and parts of containers may rocket great distances, in many directions. If material or contaminated runoff enters waterways, notify downstream users or potentially contaminated waters. Notify local health and fire officials and pollution control agencies. From a secure, explosion-proof location use water spray to cool exposed containers. If cooling streams are ineffective (venting sound increases in volume and pitch, tank discolors or shows any signs of deforming), withdraw immediately to a secure position ... The only respirators recommended for fire fighting are self-contained breathing apparatuses that have full facepieces and are operated in a pressure-demand or other positive-pressure mode.

5.2 Specific hazards arising from the chemical

This chemical is combustible. (NTP, 1992)

5.3 Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours.Avoid contacting with skin and eye. Use personal protective equipment.Wear chemical impermeable gloves. Ensure adequate ventilation.Remove all sources of ignition. Evacuate personnel to safe areas.Keep people away from and upwind of spill/leak.

6.2 Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Evacuate and restrict persons not wearing protective equipment from area of spill or leak until cleanup is complete. Remove all ignition sources. Ventilate area of spill or leak. Absorb liquids in vermiculite, dry sand, earth, peat, carbon, or a similar material and deposit in sealed containers. It may be necessary to contain and dispose of this chemical as a hazardous waste. If material or contaminated runoff enters waterways, notify downstream users of potentially contaminated waters. Contact your Department of Environmental Protection or your regional office of the federal EPA for specific recommendations.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

7.2 Conditions for safe storage, including any incompatibilities

Store in tightly closed containers in a cool, well ventilated area away from oxidizers. Metal containers involving the transfer of this chemical should be grounded and bonded. Drums must be equipped with self-closing valves, pressure vacuum bungs, and flame arresters. Use only non-sparking tools and equipment, especially when opening and closing containers of this chemical. Sources of ignition, such as smoking and open flames, are prohibited where this chemical is used, handled, or stored in a manner that could create a potential fire hazard or explosion hazard.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

8.2 Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. 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.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state	Liquid. Viscous.
Colour	Colourless.
Odour	Strong though not unpleasant aromatic odor
Melting point/freezing point	>= -34.8 - <= -24.2 °C. Atm. press.:1 atm. Remarks:Mean of three determiantions.
Boiling point or initial boiling point and boiling range	> 133.8 - < 134.3 °C. Atm. press.:1 atm.
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	39 °C. Atm. press.:995 mBar.
Auto-ignition temperature	600 °C. Atm. press.:998 mBar. Remarks:The sample does not present auto-ignition temperature behaviour until maximum test temperature 600°C.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	kinematic viscosity (in mm²/s) = 0.76. Temperature:20°C. Remarks:Kinematic viscosity.;kinematic viscosity (in mm²/s) = 0.58. Temperature:40°C. Remarks:Kinematic viscosity.;dynamic viscosity (in mPa s) = 1.01. Temperature:20°C. Remarks:Dynamic viscosity.
Solubility	less than 1 mg/mL at 68° F (NTP, 1992)
Partition coefficient n-octanol/water	log Pow = 3.7. Temperature:25 °C. Remarks:No data on pH.;Pow = 5 030. Temperature:25 °C. Remarks:No data on pH.
Vapour pressure	0.018 Pa. Temperature:25 °C. Remarks:The vapour pressure test was performed with a 20 mL/min nitrogen flow rate.
Density and/or relative density	1.336 g/mL. Temperature:20 °C.;1.336 g/mL. Temperature:20 °C.
Relative vapour density	6.24 (NTP, 1992) (Relative to Air)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Highly flammable. Insoluble in water.

10.2 Chemical stability

no data available

10.3 Possibility of hazardous reactions

FlammableP-CHLOROBENZOTRIFLUORIDE is sensitive to heat and light. This chemical reacts vigorously with oxidizing materials such as permanganates and dichromates. It is incompatible with strong bases. It is also incompatible with sodium dimethyl sulfonate. (NTP, 1992)

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Incompatibilities: strong oxidizers, such as permanganates and dichromates.

10.6 Hazardous decomposition products

When heated to decomposition it emits toxic fumes of /hydrogen chloride/ and /fluorine/.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 Rat oral 13 g/kg (13,000 mg/kg)
- Inhalation: LC50 - rat (male/female) - > 32.03 mg/L air (analytical).
- Dermal: LD50 - rabbit - > 3 300 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information

12.1 Toxicity

- Toxicity to fish: LC50 - Danio rerio (previous name: Brachydanio rerio) - 3 mg/L - 96 h.
- Toxicity to daphnia and other aquatic invertebrates: IC100 - Daphnia magna - 11.6 mg/L - 24 h.
- Toxicity to algae: EC50 - Pseudokirchneriella subcapitata (previous names: Raphidocelis subcapitata, Selenastrum capricornutum) - > 0.41 mg/L - 72 h.

- Toxicity to microorganisms: EC50 - activated sludge, domestic - 103.6 - 3 h.

12.2 Persistence and degradability

ANAEROBIC: In an anaerobic screening test with digester sludge, 64% of the 1-chloro-4-(trifluoromethyl)benzene orginally applied was degraded in 59 days(1).

12.3 Bioaccumulative potential

An estimated BCF of 110 was calculated in fish for 1-chloro-4-(trifluoromethyl)benzene(SRC), using an estimated log Kow of 3.6(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is high(SRC).

12.4 Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of 1-chloro-4-(trifluoromethyl)benzene can be estimated to be 1600(SRC). According to a classification scheme(2), this estimated Koc value suggests that 1-chloro-4-(trifluoromethyl)benzene is expected to have low mobility in soil.

12.5 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

14.1 UN Number

ADR/RID: UN2234 (For reference only, please check.)	IMDG: UN2234 (For reference only, please check.)	IATA: UN2234 (For reference only, please check.)

14.2 UN Proper Shipping Name

ADR/RID: CHLOROBENZOTRIFLUORIDES (For reference only, please check.)	IMDG: CHLOROBENZOTRIFLUORIDES (For reference only, please check.)	IATA: CHLOROBENZOTRIFLUORIDES (For reference only, please check.)

14.3 Transport hazard class(es)

ADR/RID: 3 (For reference only, please check.)	IMDG: 3 (For reference only, please check.)	IATA: 3 (For reference only, please check.)

14.4 Packing group, if applicable

ADR/RID: III (For reference only, please check.)	IMDG: III (For reference only, please check.)	IATA: III (For reference only, please check.)

14.5 Environmental hazards

ADR/RID: Yes	IMDG: Yes	IATA: Yes

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
4-chloro-α,α,α-trifluorotoluene	4-chloro-α,α,α-trifluorotoluene	98-56-6	202-681-1
European Inventory of Existing Commercial Chemical Substances (EINECS)			Listed.
EC Inventory			Listed.
United States Toxic Substances Control Act (TSCA) Inventory			Listed.
China Catalog of Hazardous chemicals 2015			Listed.
New Zealand Inventory of Chemicals (NZIoC)			Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Listed.
Korea Existing Chemicals List (KECL)			Listed.

SECTION 16: Other information

Information on revision

Creation Date	July 15, 2019
Revision Date	July 15, 2019

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

- IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home
- HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm
- IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple
- ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg
- Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp
- ECHA - European Chemicals Agency, website: https://echa.europa.eu/

Any questions regarding this SDS, Please send your inquiry to sds@xixisys.com

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