

SAFETY DATA SHEETS

According to the UN GHS revision 10

1: Identification

1.1 GHS Product identifier

Product name Tert-butyl 5-(trifluoromethyl)-1,4-diazepane-1-carboxylate

1.2 Other means of identification

Product number 1042598-29-7

Other names Tert-butyl 5-(trifluoromethyl)-1,4-diazepane-1-carboxylate

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 Zhongshan Greenrock Technology Co., Ltd.

Address No. 138, Jinsan Avenue, Sanjiao Town, Zhongshan City, Guangdong Province, China

Telephone +86-2087066781

1.5 Emergency phone number

Emergency phone number +86-2087066781

Service hours Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

2: Hazard identification

2.1 Emergency Overview

It is highly corrosive and can cause irreversible damage to the skin and eyes. If in contact, rinse immediately with plenty of water and seek medical help as soon as possible.

2.2 GHS Classification

Acute toxicity, oral : Category 4

Skin corrosion/irritation : Category 2

Serious eye damage/eye irritation : Category 2A

Specific target organ toxicity, single exposure; Respiratory tract irritation : Category 3

2.3 GHS label elements, including precautionary statements

Pictogram(s)**Signal word**

Warning

Hazard statement(s)

H302 Harmful if swallowed

H315 Causes skin irritation

H319 Causes serious eye irritation

H335 May cause respiratory irritation

Precautionary statement(s)**Prevention**

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

P264 Wash hands [and ...] thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

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

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

P264+P265 Wash hands [and ...] thoroughly after handling. Do not touch eyes.

Response

P319 Get medical help if you feel unwell.

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

P330 Rinse mouth.

P301+P317 IF SWALLOWED, Get medical help.

P302+P352 IF ON SKIN, wash with plenty of water/...

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.

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

P337+P317 If eye irritation persists, Get medical help.

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

Storage

P405 Store locked up.

Disposal

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

P501 Dispose of contents/container to ...

2.4 Physical and chemical

Acidic or alkaline substances that react with metals to produce flammable hydrogen. May cause violent exothermic reactions when in contact with other substances. At high concentrations, they have strong oxidizing or reducing properties.

2.5 Health hazards

Skin contact: May cause severe burns, tissue necrosis, and scarring. Eye contact: May cause corneal damage, vision loss, or even blindness. Inhalation of vapor or mist may cause respiratory burns and pulmonary edema.

2.6 Environmental hazards

Leakage into the environment can change the pH value of soil and water, causing serious ecological damage. It is highly toxic to aquatic organisms and can cause the death of aquatic organisms and the collapse of the ecosystem.

2.7 Other hazards which do not result in classification

3: Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
Tert-butyl 5-(trifluoromethyl)-1,4-diazepane-1-carboxylate	Tert-butyl 5-(trifluoromethyl)-1,4-diazepane-1-carboxylate	1042598-29-7	826-187-6	99%

4: First-aid measures

4.1 General advice

Stop contact immediately and remove contaminated clothing; rinse the exposed area with plenty of running water and seek medical attention immediately with the material's SDS. If the corrosive substance is acidic (such as sulfuric acid), neutralize it with a weak alkaline solution (such as 5% sodium bicarbonate) after rinsing. For alkaline corrosive substances (such as sodium hydroxide), neutralize them with a weak acidic solution (such as 1% acetic acid).

4.2 If inhaled

Move to fresh air and keep the airway open. If corrosive vapors (such as hydrochloric acid mist) are inhaled, immediately administer nebulized inhalation (normal saline + dexamethasone). If laryngeal edema or breathing difficulties occur, immediately perform a tracheotomy (requires professional operation) and seek medical attention.

4.3 In case of skin contact

Rinse with plenty of running water for 20-30 minutes (make sure to rinse thoroughly, especially between the fingers, in the armpits, and other folds). If blisters are present, do not prick them; instead, apply a sterile gauze compress (to avoid adhesion). Do not apply oily ointments to avoid affecting subsequent treatment.

4.4 In case of eye contact

Immediately flush with an eyewash or plenty of normal saline for 15-20 minutes (use a gentle flow to avoid direct exposure to the cornea); apply antibiotic eye ointment (such as erythromycin ointment) to the eyelids, wear a sterile eye patch, and seek immediate medical attention from an ophthalmologist.

4.5 If swallowed

Do not induce vomiting (to avoid secondary damage to the esophageal mucosa). If the substance is acidic, take milk or egg white orally (to protect the gastric mucosa). If the substance is alkaline, take diluted vinegar (1:10 ratio) orally. If you carry SDS, seek medical attention immediately for a gastroscopy.

4.6 Most important symptoms and effects, both acute and delayed

Acute symptoms: skin redness, swelling, blisters, ulcers, severe eye pain, photophobia, blurred vision, oral/esophageal burns, and difficulty swallowing; long-term effects: skin scarring, corneal scarring (possibly causing blindness), and esophageal stenosis.

4.7 Protection of first-aiders

Rescuers must wear corrosion-resistant chemical protective clothing, chemical protective gloves (made of fluororubber), chemical goggles and masks; stand upwind when flushing to avoid inhaling volatile corrosive gases; after contact, equipment must be cleaned with a neutralizer and then rinsed with clean water.

4.8 Notes to physician

Inform the doctor of the type of corrosive agent (acid/base), concentration, and duration of contact. Skin burns should be treated according to their depth (superficial II degree and above require skin grafting). Eye injuries should be checked for corneal epithelial integrity and, if necessary, corneal repair drugs (such as recombinant human epidermal growth factor) should be used.

5: Fire-fighting measures

5.1 Unsuitable extinguishing media

Acidic corrosive substances (such as sulfuric acid): It is strictly forbidden to use water (it releases heat when in contact with water, causing splashing) or alkaline fire extinguishing agents (it neutralizes the heat and increases the risk); Alkaline corrosive substances (such as sodium hydroxide): It is strictly forbidden to use acidic fire extinguishing agents.

5.2 Specific hazards during fire fighting

Combustion is accompanied by splashing of corrosive liquids, causing severe burns to the skin/eyes; some corrosive substances (such as nitric acid) release toxic gases when burned and also corrode fire-fighting equipment; high-temperature molten substances (such as molten alkali) easily adhere to the skin and cause deep burns.

5.3 Hazardous combustion products

Acidic corrosive substances release hydrogen chloride and sulfur dioxide (such as sulfuric acid); alkaline corrosive substances release ammonia (such as ammonia water); chlorine-containing corrosive substances release chlorine gas.

5.4 Specific extinguishing methods

Small area: Use dry powder fire extinguishing agent to put out the fire. If it is solid corrosive material, cover it with dry sand (to isolate it from the air); Large area: Cool the surrounding containers first, then use dry powder to put out the fire. It is strictly forbidden to use water directly to prevent splashing; After extinguishing the fire, use a neutralizer (weak base for acid, weak acid for alkali) to deal with the leaked material.

5.5 Special protective equipment for fire-fighters

Wear fully enclosed corrosion-resistant chemical protective clothing, chemical protective gloves (fluororubber), chemical goggles + mask; carry a pH tester (to monitor the pH value of the leak); after the operation, the equipment needs to be cleaned with a neutralizer and then rinsed with clean water.

6: Accidental release measures

6.1 Protective measures for workers

Wear fully enclosed chemical protective clothing (acid and alkali resistant), chemical protective gloves (fluororubber), chemical goggles + face mask; wear a gas mask (acid/alkali filter box) when dealing with volatile corrosive substances.

6.2 Environmental protection measure

Prevent leaked material from contacting skin or eyes; do not discharge into water or soil; treat contaminated ground with a neutralizer (sodium carbonate for acid, dilute acetic acid for alkali) until neutral.

6.3 Containment methods for leaked chemicals

Collect liquids in sealed polyethylene containers; collect solids with corrosion-resistant tools and place them in chemical-resistant bags (marked "corrosive"); store them in isolation after collection.

6.4 Cleanup methods for chemical spills

Small leakage: absorb with acid/alkali resistant cotton and then neutralize; Large leakage: transfer to storage tank with corrosion resistant pump; After cleaning, flush the ground with plenty of water (if compatible), and collect the flushing water for neutralization.

6.5 Measures to prevent the spread of leaks

Designate an 8-meter isolation zone; use corrosion-resistant isolation belts for blocking; and enhance ventilation (corrosion-resistant fans) for volatile corrosive substances.

6.6 Container leakage treatment

Minor leaks: seal with acid/alkali resistant putty; severe leaks: evacuate, have professionals transfer remaining substances, and do not reuse damaged containers.

6.7 Special considerations

In case of skin contact, rinse with an eyewash for 15 minutes; in case of eye contact, rinse with an eyewash for 15 minutes and seek medical attention; add reagents slowly during neutralization (to prevent heat release); clean protective equipment with neutralizer and then rinse with clean water.

7: Handling and storage

7.1 Safe storage conditions

Store in a corrosion-resistant warehouse (the floor is epoxy resin coated, and the walls are acid/alkali-resistant tiles); the container is made of corrosion-resistant material (glass fiber reinforced plastic for acid corrosion, high-density polyethylene for alkaline corrosion), with a capacity of ?200L to prevent dumping; the warehouse is equipped with an emergency neutralization tank (volume ?5m³) and equipped with acid/alkali neutralizers (such as sodium carbonate, dilute acetic acid).

7.2 Storage precautions

Store them separately from materials that may come into contact with the skin (such as clothing and gloves) to avoid cross contamination. Use a corrosion-resistant forklift to transport containers and avoid impact. Check the humidity in the warehouse daily (>65%) to prevent moisture from exacerbating corrosion. In case of leakage, immediately absorb it with inert materials (such as sand) and then treat it with a neutralizer.

7.3 VCI Storage Grade

Level 2 (medium-high): Metal pipes and valves are coated with VCI anti-rust paint (acid/alkali resistant type) and maintained once every six months; VCI anti-rust blocks (such as urethane) are placed in the warehouse and replenished once every quarter to prevent corrosion of metal parts.

7.4 Recommended storage temperature

5-35°F, avoid sudden temperature changes (such as moving directly from a low temperature environment to a high temperature environment); concentrated acids/bases must be kept at a temperature >30°F to prevent temperature increases from causing increased container pressure; in winter, they must be protected from freezing (temperature >5°F) to prevent the solution from freezing and cracking the container (if the label has a recommended storage temperature, follow the label).

7.5 Handling

For precautions see Safety Data Sheet section 2

Advice on safe handling : Work under hood. Do not inhale substance/mixture.

8: Exposure controls/personal protection

8.1 Respiratory protection

When exposed to corrosive vapors (such as hydrochloric acid mist and sulfuric acid mist), wear a powered air-purifying respirator (APF>50); in high-concentration environments, a positive pressure air respirator is required to avoid inhalation burns to the respiratory tract.

8.2 Recommended Filter type

For acidic corrosive substances, choose Type E filter cartridge (protects against acidic gases such as SO₂ and HCl); for alkaline corrosive substances, choose Type K filter cartridge (protects against ammonia and amines); if the product contains dust, add Type P2 filter cotton.

8.3 Eye/face protection

Wear chemical protective goggles + full-face mask. The mask must cover the chin. The lens should be made of polycarbonate (corrosion-resistant and impact-resistant). Check the sealing regularly.

8.4 Skin and body protection

Wear corrosion-resistant chemical protective clothing made of fluororubber or polytetrafluoroethylene (PTFE) to avoid direct skin contact; wear an apron (of the same material) with protection covering the chest to the knees.

8.5 Hand protection

Wear corrosion-resistant gloves. For acid corrosion, choose neoprene material; for alkaline corrosion, choose nitrile rubber material. The thickness of the gloves should be >0.5mm. Perform a water leakage test

before use.

8.6 Hygiene measures

Immediately after the operation, rinse the skin with running water for 10 minutes. If there is stinging at the contact site, apply a neutralizer (5% sodium bicarbonate for acid and 1% acetic acid for alkali) for 5 minutes. Do not use irritating skin care products to avoid aggravating skin damage.

9: Physical and chemical properties and safety characteristics

Physical state	no data available
Colour	no data available
Odour	no data available
Melting point/freezing point	no data available
Boiling point or initial boiling point and boiling range	283.3±40.0 °C(Predicted)
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	no data available
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	no data available
Partition coefficient n-octanol/water	no data available
Vapour pressure	no data available
Density and/or relative density	1.158±0.06 g/cm ³ (Predicted)
Relative vapour density	no data available
Particle characteristics	no data available

10: Stability and reactivity

10.1 Reactivity

no data available.

10.2 Chemical stability

no data available.

10.3 Possibility of hazardous reactions

no data available.

10.4 Conditions to avoid

no data available.

10.5 Incompatible materials

no data available.

10.6 Hazardous decomposition products

no data available.

11: Toxicological information

11.1 Acute toxicity

no data available

11.2 Skin corrosion/irritation

no data available

11.3 Serious eye damage/irritation

no data available

11.4 Respiratory or skin sensitization

no data available

11.5 Germ cell mutagenicity

no data available

11.6 Carcinogenicity

no data available

11.7 Reproductive toxicity

no data available

11.8 STOT-single exposure

no data available

11.9 STOT-repeated exposure

no data available

11.10 Aspiration hazard

no data available

12: Ecological information

12.1 Toxicity

no data available

12.2 Persistence and degradability

no data available

12.3 Bioaccumulative potential

no data available

12.4 Mobility in soil

no data available

12.5 Other adverse effects

no data available

13: Disposal considerations

13.1 Disposal methods for waste chemicals

Acidic corrosives can be treated with alkaline neutralizers (such as sodium carbonate) until neutralized and then disposed of as ordinary waste. Alkaline corrosives can be treated with acidic neutralizers (such as dilute hydrochloric acid) until neutralized and then disposed of. Those that cannot be neutralized must be incinerated at high temperature or chemically decomposed by a professional unit. The container must be thoroughly cleaned before being disposed of.

13.2 Precautions

Neutralization reactions must be conducted in well-ventilated, dedicated facilities, with the reaction rate controlled to prevent splashing. Disposal personnel must wear corrosion-resistant protective gear. The pH value of the neutralized waste must be controlled between 6 and 9. Direct disposal of unneutralized corrosive materials is prohibited. Emergency pools must be established at the disposal site to prevent leakage and contamination.

14: Transport information

14.1 UN Number

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

14.2 UN Proper Shipping Name

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

14.3 Transport hazard class(es)

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

14.4 Packing group, if applicable

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

14.5 Environmental hazards

ADR/RID: no data available IMDG: no data available IATA: no data available

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

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
Tert-butyl 5-(trifluoromethyl)-1,4-diazepane-1-carboxylate	Tert-butyl 5-(trifluoromethyl)-1,4-diazepane-1-carboxylate	1042598-29-7	826-187-6
Australian Inventory of Industrial Chemicals (AIIC)			Not Listed.
Catalogue of Strictly Restricted Toxic Chemicals in China			Not Listed.
China Catalog of Hazardous chemicals 2015			Not Listed.
European INventory of Existing Commercial chemical Substances			Not Listed.
IARC Monographs on the Evaluation of Carcinogenic Risks to Humans			Not Listed.
TSCA Inventory of Chemical Substances			Not Listed.

16: Other information

Information on revision

SDS Creation Date July 1, 2025

SDS Revision Date July 1, 2025

Abbreviations and acronyms in SDS

- 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%

SDS 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 Safety Data Sheet, Please send your inquiry to sales@MolBest.com

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