

SAFETY DATA SHEETS

According to the UN GHS revision 10

1: Identification

1.1 GHS Product identifier

Product name tert-Butyl 3-isothiocyanatobenzoate

1.2 Other means of identification

Product number 486415-53-6

Other names tert-Butyl 3-isothiocyanatobenzoate

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.

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Telephone +86-2087066781

1.5 Emergency phone number

Emergency phone number +86-2087066781

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2: Hazard identification

2.1 Emergency Overview

Low-risk substances usually cause only mild irritation or discomfort. Under normal handling conditions, they are unlikely to pose a significant risk to human health or the environment. However, basic safety precautions must be followed.

2.2 GHS Classification

Acute toxicity, oral; acute toxicity, dermal; acute toxicity, inhalation : Category 4

Acute toxicity, oral : Category 4

Acute toxicity, dermal : Category 4

Sensitization, Skin : Category 1, 1A, 1B

Acute toxicity, inhalation : Category 4

Sensitization, respiratory : Category 1, 1A, 1B

2.3 GHS label elements, including precautionary statements

Pictogram(s)**Signal word**

Danger

Hazard statement(s)

H302+H312+H332 Harmful if swallowed, in contact with skin or if inhaled
H302 Harmful if swallowed
H312 Harmful in contact with skin
H317 May cause an allergic skin reaction
H332 Harmful if inhaled
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled

Precautionary statement(s)**Prevention**

P233 Keep container tightly closed.
P260 Do not breathe dust/fume/gas/mist/vapors/spray.
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.
P272 Contaminated work clothing should not be allowed out of the workplace.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P284 [In case of inadequate ventilation] Wear respiratory protection.

Response

P317 Get emergency medical help.
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.
P333+P317 If skin irritation or rash occurs, Get medical help.
P342+P316 If experiencing respiratory symptoms, Get emergency medical help immediately.
P362+P364 Take off contaminated clothing and wash it before reuse.

Storage

P403 Store in a well-ventilated place.

Disposal

P501 Dispose of contents/container to ...

2.4 Physical and chemical

The physical and chemical hazards are low, and they are non-flammable, non-explosive, and non-corrosive. Some substances may be slightly flammable or irritating, but the risk is low.

2.5 Health hazards

May cause mild skin or eye irritation, such as redness and itching. Inhalation or ingestion of small amounts may cause temporary discomfort, but no serious or long-term health effects. No special medical treatment is generally required.

2.6 Environmental hazards

It has a low impact on the environment and is only slightly toxic to aquatic organisms and terrestrial ecosystems. Under normal disposal conditions, it will not cause significant environmental pollution and is highly biodegradable.

2.7 Other hazards which do not result in classification

no data available

3: Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
tert-Butyl 3-isothiocyanatobenzoate	tert-Butyl 3-isothiocyanatobenzoate	486415-53-6	-	99%

4: First-aid measures

4.1 General advice

Stop contact immediately and rinse the contact area with clean water; if symptoms are mild (such as skin redness, eye stinging), rest and observe; if symptoms persist or worsen, seek medical attention and carry the material SDS

4.2 If inhaled

Move to a ventilated place and breathe fresh air deeply; if a mild cough occurs, drink plenty of warm water to relieve it, no special treatment is required

4.3 In case of skin contact

Rinse with running water for 5-10 minutes. If itching occurs, apply anti-allergic ointment; avoid scratching

4.4 In case of eye contact

Rinse with clean water for 5 minutes and apply artificial tears; if discomfort persists, go to an ophthalmologist for treatment.

4.5 If swallowed

If a small amount is accidentally ingested (such as a mild irritant), drink plenty of water to promote excretion; seek medical attention if nausea occurs, and do not induce vomiting on your own.

4.6 Most important symptoms and effects, both acute and delayed

Mild redness and itching of the skin, brief stinging of the eyes, and a mild cough; no long-term health effects.

4.7 Protection of first-aiders

Rescuers need to wear ordinary gloves and goggles; no special heavy equipment is required, and they can just wash their hands after contact.

4.8 Notes to physician

Inform your doctor of the substance type (e.g., mild irritant, aquatic hazard); treat symptomatically (e.g., anti-allergic, anti-inflammatory); no special treatment is required.

5: Fire-fighting measures

5.1 Unsuitable extinguishing media

Mild irritants: No special contraindications, avoid using fire extinguishing agents that are incompatible with the substance (such as using alkali when encountering acid); Aquatic hazardous substances: Avoid using fire extinguishing agents that pollute water bodies (such as phosphorus-containing foam)

5.2 Specific hazards during fire fighting

The risk of combustion is low, mostly small local fires that are not easy to spread; some substances release slightly irritating gases (such as acetic acid) when burned, which have little impact on health; if the wastewater from fire extinguishing of aquatic hazardous substances enters the water body, it may harm aquatic life.

5.3 Hazardous combustion products

Carbon dioxide, water vapor, slightly irritating gases (such as sulfur dioxide, acetic acid vapor).

5.4 Specific extinguishing methods

For small areas: use dry powder/water to extinguish the fire (if compatible), and use wet cleaning for dust (to prevent dust); for large areas: use foam/water to extinguish the fire, and collect the fire extinguishing wastewater at the same time (to prevent water pollution); after extinguishing the fire, ventilate to dilute the residual gas.

5.5 Special protective equipment for fire-fighters

Wear anti-static work clothes, nitrile gloves, and goggles; wear a dust mask when working with dust; no special heavy equipment is required, and maintain good ventilation during operation.

6: Accidental release measures

6.1 Protective measures for workers

Wear anti-static work clothes, nitrile chemical-resistant gloves, and goggles; wear a dust mask or half mask when dealing with dust/volatile substances.

6.2 Environmental protection measure

Isolate the contaminated area within 5 meters; do not allow the leaked material to enter the soil/water body; ventilate/neutralize small leaks and notify the environmental protection department for large leaks.

6.3 Containment methods for leaked chemicals

Liquids are collected in plastic containers; solids are placed in sealed bags using spark-free tools; dust is collected using wet sweeping.

6.4 Cleanup methods for chemical spills

Small leakage: absorb with adsorption material and dispose of as hazardous waste; Large leakage: transfer to storage tank with compatible pump; After cleaning, rinse the ground with clean water.

6.5 Measures to prevent the spread of leaks

5-meter isolation area + signage; ventilation (ordinary fan); isolation belt to prevent spread to public areas.

6.6 Container leakage treatment

Minor leaks: Seal with sealant/tape; Serious leaks: Move to a safe area, handle professionally, and discard the container according to regulations.

6.7 Special considerations

Operators must understand the hazards of substances and first aid; protective equipment must be cleaned and stored; and the handling process must be recorded.

7: Handling and storage

7.1 Safe storage conditions

Store in a normally ventilated warehouse (natural ventilation or mechanical ventilation, air changes ? 2 times/hour); the container should be ordinary plastic or glass (such as polyethylene bottles, glass bottles) with a sealed lid; the warehouse floor should be ordinary cement with no special anti-corrosion requirements; equipped with basic fire-fighting equipment (such as fire extinguishers, fire sand).

7.2 Storage precautions

Store materials by category (e.g. liquids and solids separated) to avoid confusion; clearly mark the substance name and H code on container labels; check containers for damage monthly and clean up minor leaks immediately; eating and drinking are prohibited in the warehouse, and hands must be washed after work.

7.3 VCI Storage Grade

Level 4 (lowest): Metal containers do not require additional VCI protection and can be stored normally. The humidity in the warehouse is ?70%, which prevents slight rust on ordinary metals without affecting their use. For long-term storage (over 6 months), the dust on the surface of the container needs to be wiped off.

7.4 Recommended storage temperature

10-35?, store at room temperature; avoid extreme temperatures (below -5? or above 40?); deliquescent substances (such as certain salts) should be stored in a dry place with a desiccant (such as silica gel) and replaced regularly (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 slightly irritating dust (such as talcum powder) or vapor (such as acetic acid), wear an ordinary dust mask; a respirator is not necessary when ventilation is good.

8.2 Recommended Filter type

For dust, choose Type P1 filter cotton; for slight organic vapor, choose Type A1 filter cartridge; no composite filtration is required, basic protection is sufficient.

8.3 Eye/face protection

Wear ordinary impact-resistant goggles with resin lenses. Wear protective glasses when handling liquids to avoid splashing.

8.4 Skin and body protection

Wear ordinary work clothes (cotton or chemical fiber) and wear a waterproof apron when handling liquids to prevent clothes from getting wet.

8.5 Hand protection

Wear nitrile or latex gloves with a thickness of ≥ 0.2 mm and replace them promptly after use to avoid damage.

8.6 Hygiene measures

Wash your hands with soap and running water after work. If your skin becomes red or itchy, apply moisturizer. Do not rub your eyes with your hands. Wash your clothes normally; no special disinfection requirements are required.

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 37-40 °C

Boiling point or initial boiling 349.1±25.0 °C(Predicted)

point and boiling range

Flammability no data available

Lower and upper explosion no data available

limit/flammability limit

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- no data available

octanol/water

Vapour pressure no data available

Density and/or relative 1.08±0.1 g/cm³(Predicted)

density

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

It can be disposed of as ordinary industrial waste or recycled by a qualified unit. Liquid substances can be neutralized to a neutral pH before discharge (subject to compliance with local environmental protection standards). Solid substances can be safely landfilled or incinerated. After cleaning, the container can be recycled as ordinary waste.

13.2 Precautions

Before disposal, the characteristics of the substance must be confirmed to avoid misjudging the risk level. Mildly irritating substances must be strictly separated from food-grade waste. The disposal process must comply with local environmental regulations. Small amounts of residue can be rinsed with water, and the rinse water must be treated. Records of the amount and destination of disposal must be kept for at least three years.

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 3-isothiocyanatobenzoate	tert-Butyl 3-isothiocyanatobenzoate	486415-53-6	
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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