

SAFETY DATA SHEETS

According to the UN GHS revision 10

1: Identification

1.1 GHS Product identifier

Product name tert-Butyl 5'-hydroxy-2'-(methylthio)-6'-oxo-6'H-spiro[cyclohexane-1,9'-pyrazino[1',2':1,5]pyrrolo[2,3-d]pyrimidine]-7'(8'H)-carboxylate

1.2 Other means of identification

Product number 2170746-97-9

Other names tert-Butyl 5'-hydroxy-2'-(methylthio)-6'-oxo-6'H-spiro[cyclohexane-1,9'-pyrazino[1',2':1,5]pyrrolo[2,3-d]pyrimidine]-7'(8'H)-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

Flammable material. Contact with ignition sources may cause fire. Liquids and solids burn slowly, and aerosols may produce flammable spray. Keep away from heat and ignition sources.

2.2 GHS Classification

Flammable solids : Category 1

Flammable solids : Category 2

Self-heating substances and mixtures : Category 2

2.3 GHS label elements, including precautionary statements

Pictogram(s)**Signal word**

Danger

Hazard statement(s)

H228 Flammable solid

H252 Self-heating in large quantities; may catch fire

Precautionary statement(s)**Prevention**

P210 Keep away from heat, hot surface, sparks, open flames and other ignition sources. No smoking.

P235 Keep cool.

P240 Ground/bond container and receiving equipment.

P241 Use explosion-proof [electrical/ventilating/lighting/.../] equipment.

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

Response

P370+P378 In case of fire, Use ... to extinguish.

Storage

P407 Maintain air gap between stacks or pallets.

P410 Protect from sunlight.

P413 Store bulk masses greater than ... kg/...lbs at temperatures not exceeding ... °C/...°F.

P420 Store separately.

Disposal

no data available

2.4 Physical and chemical

Flammable liquid with a flash point between 23-60°C. It burns easily when exposed to heat or open flame. Flammable solid: May ignite when exposed to heat, friction, or impact. Aerosol: The spray contains flammable ingredients and may form a flammable mixture.

2.5 Health hazards

The primary hazard is burns from fire. Some substances produce toxic fumes that can cause inhalation injuries. Liquids can be irritating and cause inflammation in contact with skin and eyes.

2.6 Environmental hazards

Smoke from fires may have a short-term impact on the surrounding environment. Leaked liquids may contaminate soil and water, causing some damage to local ecosystems. Most substances are naturally degradable in the environment.

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
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tert-Butyl 5'-hydroxy-2'-(methylthio)-6'-oxo-6'H-spiro[cyclohexane-1,9'-pyrazino[1',2':1,5]pyrrolo[2,3-d]pyrimidine]-7'(8'H)-carboxylate	tert-Butyl 5'-hydroxy-2'-(methylthio)-6'-oxo-6'H-spiro[cyclohexane-1,9'-pyrazino[1',2':1,5]pyrrolo[2,3-d]pyrimidine]-7'(8'H)-carboxylate	2170746-97-9	863-539-8	99%
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4: First-aid measures

4.1 General advice

Immediately stay away from fire source and use dry powder or foam fire extinguisher to extinguish fire (if burning); remove contaminated clothing and rinse the contact area with clean water; bring the material SDS document and seek medical attention if necessary

4.2 If inhaled

Move to a ventilated area. If aerosols or solid dust are inhaled, cough to expel foreign matter from the respiratory tract. If mild chest tightness occurs, rest and observe. If symptoms persist, seek medical attention.

4.3 In case of skin contact

Rinse with running water for 10-15 minutes. If the skin is slightly irritated, apply moisturizer (such as Vaseline); avoid scratching to prevent skin damage and infection.

4.4 In case of eye contact

Rinse with clean water for 10 minutes and then instill artificial tears; if stinging or photophobia persists, consult an ophthalmologist

4.5 If swallowed

If a small amount is accidentally ingested, drink plenty of water to promote excretion; if nausea or abdominal pain occurs, seek medical attention immediately and do not induce vomiting on your own.

4.6 Most important symptoms and effects, both acute and delayed

Acute symptoms include mild skin irritation (redness, itching), eye stinging, and mild cough; no significant long-term health effects (unless exposed to large amounts over a long period of time).

4.7 Protection of first-aiders

Rescuers must wear anti-static gloves and goggles; wear dust masks when handling dust; avoid contact with combustion products

4.8 Notes to physician

Inform the doctor of the substance type and exposure amount; treat symptoms (eg. antihistamine ointment for skin irritation, anti-inflammatory eye drops for eye irritation).

5: Fire-fighting measures

5.1 Unsuitable extinguishing media

Flammable liquids (flash point 23-60°C): Avoid using high-pressure water (diffusing liquids); Flammable solids: Do not use water (some solids release heat when in contact with water, such as sulfur); Aerosols: Do not squeeze leaking tanks (explosion prevention).

5.2 Specific hazards during fire fighting

The combustion of flammable liquids produces a large amount of vapor, which can easily form a flowing fire; the combustion of flammable solids can easily produce toxic smoke and dust (such as plastics); aerosol cans can easily rupture and explode when heated, spraying flames.

5.3 Hazardous combustion products

Carbon monoxide, carbon oxides, organic vapors (such as benzene, toluene); combustion of some solids releases hydrogen chloride and cyanide (when containing chlorine/cyanide components).

5.4 Specific extinguishing methods

Flammable liquids: Use dry powder/foam (ordinary foam) for small areas, and cover large areas with foam + firebreaks to intercept (to prevent flow); Flammable solids: Cover with dry powder/dry sand to avoid wind (to prevent dust from intensifying combustion); Aerosols: Remove surrounding fire sources before extinguishing the fire, use dry powder to extinguish the fire, and it is strictly forbidden to touch the leaking tank.

5.5 Special protective equipment for fire-fighters

Wear fire-resistant clothing, chemical-resistant gloves, and a half-mask respirator (equipped with a vapor filter cartridge); carry a temperature detector (to monitor the tank temperature); and maintain a safe distance of 10 meters from the fire scene during operation.

6: Accidental release measures

6.1 Protective measures for workers

Wear anti-static work clothes, anti-static gloves, and chemical goggles; wear a gas mask (organic vapor filter cartridge) for gases/volatile liquids; wear impact protection for aerosols.

6.2 Environmental protection measure

Liquids/aerosols are prevented from flowing into sewers/rivers, and oil booms + oil absorbent cotton are used to pollute water bodies; gas leaks are monitored for concentration to prevent them from spreading to residential areas; solids are prevented from dust polluting the soil.

6.3 Containment methods for leaked chemicals

Gas: Shut off the leak source (when safe), and use explosion-proof fan to lead the leak to an open area; Liquid: Collect in anti-static container; Solid: Put non-sparking tools into anti-static container; Aerosol: Collect the leaked tank (no squeezing).

6.4 Cleanup methods for chemical spills

Liquid: absorb with a small amount of oil-absorbing cotton and transfer with a large amount of explosion-proof pump; Solid: transfer with spark-free tools (to prevent friction); Aerosol: leaking tanks are collected separately and disposed of professionally.

6.5 Measures to prevent the spread of leaks

Designate a 10-meter isolation zone and prohibit open flames/static equipment; set up fire barriers for liquids and anti-static isolation belts for gases; use explosion-proof ventilation to reduce concentration (explosion limit).

6.6 Container leakage treatment

Gas: Minor leaks should be sealed with anti-static sealant, serious leaks should be transferred after pressure relief; Liquid: Anti-static sealant should be used to seal, serious leaks should be transferred with explosion-proof pump; Aerosol: Do not squeeze, wrap in sealed bag.

6.7 Special considerations

Eliminate static electricity before operation; provide good ventilation to prevent gas accumulation; perform anti-static testing on tools; clean protective equipment and perform anti-static testing after leak treatment.

7: Handling and storage

7.1 Safe storage conditions

Store in a normally ventilated warehouse (air changes ? 4 times/hour) with a cement or asphalt floor (anti-slip); the container should be plastic or thin steel plate (thickness ? 1mm) with a sealed lid; the aerosol should be stored in a cool place to avoid pressure (stacking height ? 1.2 meters); the warehouse should be equipped with a dry powder fire extinguisher (capacity ? 2kg).

7.2 Storage precautions

Store away from oxidants (isolation distance ? 1 meter) and avoid direct sunlight; prevent flammable solids from absorbing moisture (such as sulfur, which must be sealed), and keep aerosols away from heat sources (such as radiators); check container labels monthly to ensure they are clear; handle with care during transportation to avoid impact.

7.3 VCI Storage Grade

Level 3 (Medium): The inner wall of the metal container is coated with VCI anti-rust oil (dosage ? 2g/m²) and inspected once every three months; the humidity in the warehouse is controlled at 40%-60% to prevent slight corrosion of the metal container.

7.4 Recommended storage temperature

10-35?, flammable liquids with a flash point ?23? can be relaxed to 5-40?; aerosols must be ?30? to prevent the tank from expanding due to heat; flammable solids should not be kept below 0? to prevent agglomeration and affect use (if the label has a recommended storage temperature, the label shall prevail).

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 flammable liquids with medium flash points (such as kerosene) or dusts (such as sulfur), wear a half-mask filtering respirator (APF?5); upgrade to a powered air respirator when ventilation is poor.

8.2 Recommended Filter type

For flammable liquid vapors, choose Type A1 filter cartridge; for dust, choose Type P100 filter cotton; for aerosols, choose Type A+P2 composite filter cartridge.

8.3 Eye/face protection

Wear ordinary impact-resistant goggles. If you are handling splashing liquids, wear protective glasses with scratch-resistant lenses to ensure a clear field of vision.

8.4 Skin and body protection

Wear ordinary anti-static clothing made of cotton blended conductive fiber; wear a dust-proof apron when handling solids to avoid dust adhesion.

8.5 Hand protection

Wear nitrile chemical-resistant gloves with a thickness of ?0.3mm and a certain degree of wear resistance. Check for damage after use.

8.6 Hygiene measures

Wash your hands with clean water after work. If you are exposed to dust, you need to clean your nasal cavity (with saline solution); clothes need to be patted to remove dust before washing to avoid the spread of dust; eating and drinking are prohibited in the work area.

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	no data available
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	no data available
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

Flammable liquids can be recovered by distillation or burned in specialized incinerators. Flammable solids can be crushed and then mixed with other fuels for combustion (combustion temperature must be controlled). Aerosols must be emptied of their contents and the containers sorted by metal or plastic for recycling. Residues must be disposed of as flammable waste.

13.2 Precautions

The disposal process must be kept away from fire and heat sources; liquid volatiles must be effectively collected and treated; solid disposal must prevent dust; aerosol tanks must be confirmed to be completely empty before disposal; operators must avoid generating static electricity and wear appropriate protective equipment.

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'-hydroxy-2'-(methylthio)-6'-oxo-6'H-spiro[cyclohexane-1,9'-pyrazino[1',2':1,5]pyrrolo[2,3-d]pyrimidine]-7'(8'H)-carboxylate	tert-Butyl 5'-hydroxy-2'-(methylthio)-6'-oxo-6'H-spiro[cyclohexane-1,9'-pyrazino[1',2':1,5]pyrrolo[2,3-d]pyrimidine]-7'(8'H)-carboxylate	2170746-97-9	863-539-8
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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