

SAFETY DATA SHEETS

According to the UN GHS revision 10

1: Identification

1.1 GHS Product identifier

Product name 3-[4-(morpholin-4-yl)-7H-pyrrolo[2,3-d]pyrimidin-5-yl]benzotrile

1.2 Other means of identification

Product number 1527473-33-1

Other names 3-[4-(morpholin-4-yl)-7H-pyrrolo[2,3-d]pyrimidin-5-yl]benzotrile

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

Highly toxic substances, even small amounts of which can cause death or serious health effects. They can enter the body through inhalation, skin contact, or ingestion. Immediate protective measures must be taken to avoid any contact.

2.2 GHS Classification

Acute toxicity, oral : Category 3

2.3 GHS label elements, including precautionary statements

Pictogram(s)

Signal word	Danger
Hazard statement(s)	H301 Toxic if swallowed
Precautionary statement(s)	
Prevention	P264 Wash hands [and ...] thoroughly after handling. P270 Do not eat, drink or smoke when using this product.
Response	P321 Specific treatment (see ... on this label). P330 Rinse mouth. P301+P316 IF SWALLOWED,Get emergency medical help immediately.
Storage	P405 Store locked up.
Disposal	P501 Dispose of contents/container to ...

2.4 Physical and chemical

Some substances may also be flammable or corrosive. Mixing with other substances may produce toxic products. Highly volatile substances can form toxic vapor clouds, expanding the hazard range.

2.5 Health hazards

Acute toxicity,May cause respiratory failure, cardiac arrest, nervous system depression, or organ failure. Severe symptoms may appear within a short period of exposure (minutes to hours). Long-term effects may include permanent organ damage.

2.6 Environmental hazards

It is extremely toxic to aquatic organisms and terrestrial ecosystems, and even a small release can cause large-scale biological mortality. It may persist in the environment and accumulate through the food chain, causing long-term damage to ecosystems.

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
3-[4-(morpholin-4-yl)-7H-pyrrolo[2,3-d]pyrimidin-5-yl]benzotrile	3-[4-(morpholin-4-yl)-7H-pyrrolo[2,3-d]pyrimidin-5-yl]benzotrile	1527473-33-1	808-609-0	99%

4: First-aid measures

4.1 General advice

Stop contact immediately and move to a safe area; bring the material SDS document and call emergency services immediately; record the route of exposure (inhalation/skin/ingestion), exposure time and dosage for the doctor's judgment.

4.2 If inhaled

Quickly transfer the patient to a place with fresh air, keep the patient lying flat with the head tilted to one side (to prevent suffocation by vomitus); if cyanosis or breathing difficulties occur, immediately give oxygen (flow rate 5-10L/min); it is strictly forbidden to feed/drink water to the unconscious person, and seek medical attention immediately.

4.3 In case of skin contact

Immediately remove contaminated clothing (if clothing is stuck to the skin, cut it with scissors to avoid tearing it). Rinse the affected area with plenty of running water for 20-30 minutes (the water temperature should be around 37°C, avoiding excessive heat or cold). If the skin is damaged, cover it with sterile gauze after rinsing. Do not apply ointment.

4.4 In case of eye contact

Immediately flush with an eyewash station for 15 minutes (open the eyelids to ensure thorough flushing of the upper and lower fornixes); wear a light-shielding eye mask after flushing to avoid strong light stimulation, and immediately seek medical attention from an ophthalmologist (bring along the substance SDS).

4.5 If swallowed

Self-induced vomiting is strictly prohibited (especially with corrosive and toxic substances, which may cause secondary burns to the esophagus). If the patient is conscious and not convulsing, they can drink 50-100ml of milk under the guidance of a doctor (to protect the gastric mucosa).

4.6 Most important symptoms and effects, both acute and delayed

Acute symptoms: nausea and vomiting, abdominal pain, dyspnea, convulsions, confusion, and decreased blood pressure; delayed symptoms: liver and kidney damage (appearing within 24-72 hours), methemoglobinemia (such as nitrite poisoning).

4.7 Protection of first-aiders

Rescuers must wear fully enclosed chemical protective clothing, a gas mask (with a targeted gas filter cartridge, such as for organic vapors and acid gases), and chemical protective gloves; avoid direct contact with the patient's vomitus/secretions, and wash hands immediately with chlorine-containing disinfectant after contact.

4.8 Notes to physician

Inform the physician of the substance's toxicity (e.g., oral LD50 = 5 mg/kg) and route of exposure; prioritize gastric lavage (physician evaluation required for appropriateness) and administer antidotes (e.g., atropine for organophosphate poisoning); monitor liver and kidney function, electrolytes, and coagulation function.

5: Fire-fighting measures

5.1 Unsuitable extinguishing media

It is strictly forbidden to use fire extinguishing agents that may cause the spread of toxic substances (such as high-pressure water jets); if flammable liquids are involved, avoid using carbon dioxide (which may cause toxic vapor condensation).

5.2 Specific hazards during fire fighting

Combustion may be accompanied by the release of highly toxic substances (such as cyanide and arsenide), which are fatal by inhalation or skin contact; the combustion of flammable components can easily cause explosions and intensify the spread of toxic substances; toxic vapors are heavier than air and tend to accumulate in low-lying areas.

5.3 Hazardous combustion products

Highly toxic gases (such as hydrogen chloride, hydrogen fluoride, phosgene), carbon monoxide, nitrogen oxides; some contain heavy metal components that release toxic fumes such as mercury and lead.

5.4 Specific extinguishing methods

For small areas: use dry powder fire extinguishing agent to extinguish the fire, and dilute the toxic vapor with mist water (avoid direct spraying); for large areas: give priority to evacuation. If fire extinguishing is necessary, set up a fire extinguishing point upwind and cover it with foam (to isolate oxygen); after extinguishing the fire, test the area for toxicity concentration (entry is allowed only when the value is below MAC).

5.5 Special protective equipment for fire-fighters

Wear fully enclosed chemical protective clothing, gas masks (with targeted gas filter boxes, such as organic vapor + acidic gas), and chemical protective gloves (made of fluororubber); carry a portable toxic gas detector; equipment must be disinfected after the operation, and personnel must undergo health monitoring.

6: Accidental release measures

6.1 Protective measures for workers

Wear fully enclosed chemical protective clothing, positive pressure air respirator, chemical protective gloves (toxic-resistant type) and goggles; avoid direct contact with the skin and wash immediately after work.

6.2 Environmental protection measure

Isolate the 30-meter contaminated area to prevent the leak from spreading through rainwater/groundwater; take samples of water/soil for testing, and use activated carbon adsorption (organic poison) or neutralizer (inorganic poison) for treatment when exceeding the standard; strictly prohibit the leak from entering the drinking water source.

6.3 Containment methods for leaked chemicals

Collect liquids in corrosion-resistant sealed containers (marked with "toxic substances"); collect solids in chemical-resistant bags (to avoid dust); and store them separately in a hazardous waste warehouse after collection, away from food/feed.

6.4 Cleanup methods for chemical spills

Small leakage: absorb with special absorbent cotton (toxic-resistant) and put into chemical-proof bag; large leakage: professionals use chemical-proof pump to transfer to special storage tank; after cleaning, treat the ground with neutralizer (weak base for acid poison and weak acid for alkali poison).

6.5 Measures to prevent the spread of leaks

Set up a 30-meter isolation zone and prohibit unauthorized personnel from entering; volatile toxic substances require explosion-proof ventilation to reduce gas concentration; use chemical defense isolation belts to block them, and focus on monitoring low-lying areas (to prevent the accumulation of toxic substances).

6.6 Container leakage treatment

Minor leaks: Seal with compatible sealant; Serious leaks: Evacuate immediately, close the upstream valve (if safe), and have the toxic material disposal team handle it. It is strictly forbidden to open the container without authorization.

6.7 Special considerations

Workers must receive poisoning first aid training and carry antidotes (if applicable). In case of skin contact, flush immediately with plenty of water for 15 minutes. In case of inhalation poisoning, move immediately to fresh air and seek medical attention.

7: Handling and storage

7.1 Safe storage conditions

Store in a closed, impermeable dedicated warehouse (the walls are made of anti-corrosion materials, such as polyethylene coating); the container is made of corrosion-resistant material (such as polytetrafluoroethylene, glass-lined steel), with a double sealing cover (threaded cover + nitrile rubber sealing ring); the warehouse is equipped with a negative pressure ventilation system (air changes ? 8 times/hour), and the exhaust gas must be treated with activated carbon adsorption (adsorption efficiency ? 95%).

7.2 Storage precautions

Store them separately from food, feed, and medicine (isolation distance ? 3 meters), and strictly prohibit them from being adjacent to drinking water sources; clearly mark "highly toxic" and H code on container labels and store them separately on locked shelves; check the sealing of containers weekly and immediately transfer them to the emergency treatment area if any leakage is found; workers must wear fully enclosed chemical protective clothing before entering the warehouse.

7.3 VCI Storage Grade

Level 1 (highest): The inner wall of the metal container is coated with a VCI anti-rust coating (thickness ? 50?m), and the outer surface of the container is wrapped with a vapor phase anti-rust film; the concentration of toxic substances in the warehouse is tested monthly to ensure that it is lower than the

MAC value (for example, MAC of oral toxic substances $\geq 0.1\text{mg}/\text{m}^3$).

7.4 Recommended storage temperature

10-30°C, avoid extreme temperatures (below 0°C or above 35°C); volatile toxic substances must be kept at a temperature $\approx 25^\circ\text{C}$ to reduce vapor release; refrigerated storage substances (such as certain biotoxins) must be maintained at 2-8°C and equipped with dual power supply protection (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

Choose according to the exposure route: volatile substances require positive pressure air respirators; dust/aerosols require powered air-purifying respirators to ensure the protection factor (APF) ≥ 1000 .

8.2 Recommended Filter type

For organic toxic substances, choose Type A filter cartridge (to protect against organic vapors, such as benzene and methanol); for inorganic toxic substances, choose Type B (to protect against ammonia) or Type E (to protect against acidic gases, such as hydrogen chloride); for dust, add Type P3 filter cotton.

8.3 Eye/face protection

Wear a full-face chemical protective mask. The mask material must be resistant to toxic penetration (such as fluororubber), and the lens must be anti-fog and anti-chemical corrosion.

8.4 Skin and body protection

Wear fully enclosed chemical protective clothing. The material must be compatible with toxic substances (such as polyethylene + neoprene composite material); the cuffs and ankles must be tightened and equipped with emergency escape zippers.

8.5 Hand protection

Wear toxic and chemical-resistant gloves, preferably made of fluororubber or butyl rubber, with a length of ≥ 30 cm, covering the forearm, and change every 4 hours

8.6 Hygiene measures

Immediately after the operation, clean the skin with a special detergent (such as a weak alkaline detergent), and then rinse with running water for 15 minutes; clothes need to be disinfected at high temperature (above 60°C) before washing; regular physical examinations (blood routine, liver and kidney function tests every 3 months).

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	>223°C (dec.)
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	DMSO: soluble 10mg/mL, clear
Partition coefficient n-octanol/water	no data available
Vapour pressure	no data available
Density and/or relative density	1.4±0.1 g/cm ³
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

This must be handled by a qualified unit that handles highly toxic waste, using high-temperature incineration (800-1000°C) or chemical neutralization (such as oxidative decomposition) to completely destroy the toxicity. Liquid highly toxic substances must be solidified before incineration. Those that cannot be incinerated must be stabilized/solidified before being safely landfilled.

13.2 Precautions

Disposal personnel must wear fully enclosed chemical protective suits and positive pressure respirators; waste must be strictly classified and packaged to prevent leakage; exhaust gas and wastewater generated during the disposal process must meet discharge standards; mixing with other types of waste is prohibited; and disposal records must be kept for at least 10 years for traceability.

14: Transport information

14.1 UN Number

ADR/RID: 2811

IMDG: 2811

IATA: 2811

14.2 UN Proper Shipping Name

ADR/RID: no data available

IMDG: no data available

IATA: no data available

14.3 Transport hazard class(es)

ADR/RID: no data available

IMDG: no data available

IATA: no data available

14.4 Packing group, if applicable

ADR/RID: no data available

IMDG: no data available

IATA: no data available

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
3-[4-(morpholin-4-yl)-7H-pyrrolo[2,3-d]pyrimidin-5-yl]benzotrile	3-[4-(morpholin-4-yl)-7H-pyrrolo[2,3-d]pyrimidin-5-yl]benzotrile	1527473-33-1	808-609-0
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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