

Shanghai Aladdin Biochemical Technology Co., Ltd.
No. 809, Chuhua Branch Road, Fengxian District, Shanghai

SAFETY DATA SHEET

Version: v1
Revision Date: 2024-02-11
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : 1-[3,5-bis(trifluoromethyl)phenyl]-3-[(S)-[(1S,2S,4S,5R)-5-ethenyl-1-azabicyclo[2.2.2]octan-2-yl](6-methoxyquinolin-4-yl)methyl]thiourea
Product Number : B177656
Brand : aladdin
CAS-No. : 852913-16-7

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Manufacture of substances.

1.3 Details of the supplier of the safety data sheet

Company : Shanghai Aladdin Biochemical Tech Co., Ltd
Address : 36 Xinjinqiao Road, Shanghai
Telephone : 400-620-6333
Fax : no data available

1.4 Emergency telephone number


Emergency Phone : 0532-83889090

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Acute toxicity, oral (Category 3), H301

2.2 GHS Label elements, including precautionary statements

Pictogram	
Signal word	Danger
Hazard statement(s)	
H301	Toxic if swallowed
Precautionary statement(s)	
P264	Wash hands [and ...] thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P321	Specific treatment (see ... on this label).
P330	Rinse mouth.

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P301+P310	IF SWALLOWED: Immediately call a POISON CENTER/doctor/...
P405	Store locked up.
P501	Dispose of contents/container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms	: 1-[3,5-bis(trifluoromethyl)phenyl]-3-((S)-(6-methoxy-4-quinolinyl)-[(2S,4S,5R)-5-ethylene 1-aza-bicyclo[2.2.2]oct-2-yl)methyl]thiourea; epi-N-quinolinyl-N'-bis(3,5-trifluoromethyl)phenylsulfide Urea
Formula	: C ₂₉ H ₂₈ F ₆ N ₄ O ₅
Molecular weight	: 594.62
CAS No.	: 852913-16-7
EC-NO.	: no data available

Component	Classification	Concentration
1-[3,5-bis(trifluoromethyl)phenyl]-3-((S)-[(1S,2S,4S,5R)-5-ethenyl-1-azabicyclo[2.2.2]octan-2-yl](6-methoxyquinolin-4-yl)methyl]thiourea	no data available	97%

SECTION 4: First aid measures

4.1 Description of first aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

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.

In case of skin contact

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

In case of eye contact

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

If swallowed

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.

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4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

no data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Unsuitable extinguishing media

no data available

5.2 Special hazards arising from the substance or mixture

Carbon oxides Nitrogen oxides (NOx) Sulfur oxides Hydrogen fluoride

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

no data available

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

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

6.4 Reference to other sections

For disposal see section 13.

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SECTION 7: Handling and storage

7.1 Precautions for safe handling

Operators should be specially trained and strictly abide by the operating procedures. Operation and disposal should be carried out in a place with local ventilation or general ventilation facilities. Avoid eye and skin contact and avoid breathing vapor. See Section 8 for personal protective measures. Keep away from fire and heat sources, and smoking is strictly prohibited in the workplace. Use explosion-proof ventilation systems and equipment. If canning is required, the flow rate should be controlled, and there should be a grounding device to prevent the accumulation of static electricity. Avoid contact with incompatible substances such as oxidizing agents (see section 10 for incompatible substances). When handling, it should be lightly loaded and unloaded to prevent damage to packaging and containers. Empty containers may be harmful residues. Wash hands after use and prohibit eating or drinking in the workplace. Equipped with the corresponding variety and quantity of fire fighting equipment and leakage emer

7.2 Conditions for safe storage, including any incompatibilities

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Store under inert gas.

7.3 Specific end use(s)

no data available

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. The selected protective gloves have to satisfy the specifications of Regulation (EU)2016/425 and the standard EN 374 derived from it.

Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a fullface particle respirator type

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N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN(EU).

Control of environmental exposure

If safety requires, prevent further leakage or spillage. Do not let the product enter the sewer.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	form: powder to crystalline color: White to brown
b) Odour	no data available
c) Odour Threshold	no data available
d) pH	no data available
e) Melting point/freezing point	no data available
f) Initial boiling point and boiling range	no data available
g) Flash point	no data available
h) Evaporation rate	no data available
i) Flammability (solid, gas)	no data available
j) Upper/lower flammability or explosive limits	no data available
k) Vapour pressure	no data available
l) Vapour density	no data available
m) Relative density	no data available
n) Water solubility	no data available
o) Partition coefficient: n-octanol/water	no data available
p) Auto-ignition temperature	no data available
q) Decomposition temperature	no data available
r) Viscosity	no data available
s) Explosive properties N	no data available
t) Oxidizing properties N	no data available

9.2 Other safety information

no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

no data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

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no data available

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Acute toxicity estimate Oral - 200 mg/kg

Skin corrosion/irritation

no data available

Serious eye damage/eye irritation

no data available

Respiratory or skin sensitisation

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

Specific target organ toxicity - single exposure

no data available

Specific target organ toxicity - repeated exposure

no data available

Aspiration hazard

no data available

Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity

no data available

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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 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

no data available

SECTION 13:

13.1 Disposal considerations

Product

Recycle to process, if possible. Consult your local regional authorities and an expert of disposal. You may be able to dissolve or mix material with a combustible solvent and little by little burn in a chemical incinerator equipped with an afterburner and scrubber system. If a large amount of the substance is burned at a time, an explosion may occur.

Observe all federal, state and local regulations when disposing of the substance.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

DOT (US)

UN number: 2811

Packing group: III

Class: 6.1

Proper shipping name: TOXIC SOLID,

Reportable Quantity(RQ): no data

Poison Inhalation Hazard: no data

ORGANIC, N.O.S. (N-(3,5-

available

available

Bis(trifluoromethyl)phenyl)-N'-((8 α ,9S)-

6'- methoxy-9-cinchoanyl)thiourea)

Environmental Hazards: no

IMDG

UN number: 2811

Packing group: III

EMS-No: no data available

Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (N-(3,5-Bis(trifluoromethyl)phenyl)-N'-((8 α ,9S)-6'- methoxy-9-cinchoanyl)thiourea)

IATA

UN number: 2811

Packing group: III

Class: 6.1

Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (N-(3,5-Bis(trifluoromethyl)phenyl)-N'-((8 α ,9S)-6'- methoxy-9-cinchoanyl)thiourea)

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SECTION 15: Regulatory information

This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.

SECTION 16: Other information

Further information

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