

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 : tert-Butyl 5-cyano-3-iodo-1H-indole-1-carboxylate
Product Number : T195404
Brand : aladdin
CAS-No. : 864685-26-7

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)

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute oral toxicity Category 4

Acute dermal toxicity Category 4

Acute Inhalation Toxicity - Dusts and Mists Category 4

Skin Corrosion/Irritation Category 2

Serious Eye Damage/Eye Irritation Category 2

Specific target organ toxicity (single exposure) Category 3

Target Organs - Respiratory system.

2.2 GHS Label elements, including precautionary statements

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Pictogram	no data available
Signal word	Warning
Hazard statement(s)	
H315	Causes skin irritation
H319	Causes serious eye irritation
H335	May cause respiratory irritation
H302+H312+H332	Harmful if swallowed, in contact with skin or if inhaled
Precautionary statement(s)	
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.
P312	Call a POISON CENTER or doctor/... if you feel unwell.
P330	Rinse mouth.
P301+P312	IF SWALLOWED: call a POISON CENTER/doctor/... IF you feel unwell.
P302+P350	IF ON SKIN: Gently wash with plenty of soap and 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+P313	IF SKIN irritation occurs: Get medical advice/attention.
P362+P364	Take off contaminated clothing and wash it before reuse.
P501	Dispose of contents/container to an approved waste disposal plant.

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

None identified

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms	: no data available
Formula	: C ₁₄ H ₁₃ IN ₂ O ₂
Molecular weight	: 368.17
CAS No.	: 864685-26-7
EC-NO.	: no data available

Component	Classification	Concentration
tert-Butyl 5-cyano-3-iodo-1H-indole-1-carboxylate		
	no data available	98%

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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

Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.

In case of skin contact

Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.

In case of eye contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required. Keep eye wide open while rinsing.

If swallowed

Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.

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

Water, Foam, Carbon dioxide (CO₂), Dry powder

Unsuitable extinguishing media

no data available

5.2 Special hazards arising from the substance or mixture

no data available

5.3 Advice for firefighters

wear self-contained breathing and full protective gear.

5.4 Further information

Use water spray to cool unopened containers.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Ensure adequate ventilation. Use personal protective equipment as required.

6.2 Environmental precautions

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Do not flush into surface water or sanitary sewer system. Do not allow material to contaminate ground water system. Prevent product from entering drains. Local authorities should be advised if significant spillages cannot be contained.

6.3 Methods and materials for containment and cleaning up

Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed Up containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Avoid dust formation. Avoid contact with skin, eyes or clothing. Avoid ingestion and inhalation.

7.2 Conditions for safe storage, including any incompatibilities

Keep containers tightly closed in a dry, cool and well-ventilated place.

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.

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Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a fullface particle respirator type 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	no data available
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.

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10.3 Possibility of hazardous reactions

no data available

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x), Hydrogen cyanide²(hydrocyanic acid), Hydrogen iodide

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

no data available

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

no data available

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

no data available

12.6 Other adverse effects

no data available

SECTION 13:

13.1 Disposal considerations

Product

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste.

Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

DOT (US)

UN number: UN3439

Packing group: no data available

Class: no data available

Proper shipping name: no data available

Reportable Quantity(RQ): no data available

Poison Inhalation Hazard: no data available

Environmental Hazards: no data available

IMDG

UN number: UN3439

Packing group: no data available

EMS-No: no data available

Proper shipping name: no data available

IATA

UN number: UN3439

Packing group: no data available

Class: no data available

Proper shipping name: no data available

SECTION 15: Regulatory information

Please note that waste disposal should also meet local regulations. If applicable, the chemical meets the requirements of the Regulations on the Safety Management of Hazardous Chemicals (adopted by the State Council

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on December 4, 2013).

SECTION 16: Other information

Further information

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