

Classified as hazardous in accordance with the criteria of EPA New Zealand

Section 1 - Identification

Product Identifier

Product Name	<u>1-Boc-3-iodoindole-5-carbonitrile</u>
CAS No	864685-26-7
Molecular Formula	C ₁₄ H ₁₃ IN ₂ O ₂
Molecular Weight	368.17
Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

Product Code	H64169
Address	Thermo Fisher Scientific New Zealand Ltd 244 Bush Road, Albany, Auckland, New Zealand
Emergency Tel.	CHEMTREC® 09 980 6780 or +64 9 980 6780
Telephone / Fax Numbers	Tel: 09 980 6700 Fax: 09 980 6788
E-mail address	<u>ANZinfo@thermofisher.com</u>

Section 2 - Hazard(s) Identification

Classification under Work Safe New Zealand

Classified as hazardous in accordance with the criteria of EPA New Zealand

GHS Classification

Physical hazards

Based on available data, the classification criteria are not met

Health hazards

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

Environmental hazards

Based on available data, the classification criteria are not met

Label Elements

**Signal Word****Warning****Hazard Statements**

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 Statements**Prevention**

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray

P264 - Wash face, hands and any exposed skin 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

Response

P302 + P352 - IF ON SKIN: 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

P312 - Call a POISON CENTER or doctor if you feel unwell

P330 - Rinse mouth

P362 + P364 - Take off contaminated clothing and wash it before reuse

Storage

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

Other hazards which do not result in classification

Section 3 - Composition and Information on Ingredients

Component	CAS No	Weight %
1-Boc-3-iodoindole-5-carbonitrile	864685-26-7	<=100

Section 4 - First Aid Measures

Description of first aid measures**General Advice**

If symptoms persist, call a physician.

New Zealand Emergency Tel.CHEMTREC®
09 980 6780 or +64 9 980 6780**Inhalation**

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

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
Ingestion	Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.
Self-Protection of the First Aider	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.
First Aid Facilities	Eyewash, safety shower and washroom.
Most important symptoms and effects	None reasonably foreseeable.
Notes to Physician	Treat symptomatically.

Section 5 - Fire Fighting Measures

Suitable Extinguishing Media

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

Extinguishing media which must not be used for safety reasons

No information available.

Specific Hazards Arising from the Chemical

Thermal decomposition can lead to release of irritating gases and vapors.

Hazardous Combustion Products

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

Special protective equipment and precautions for fire fighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

Section 6 - Accidental Release Measures

Personal Precautions, Protective Equipment and Emergency Procedures

Emergency procedures

Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.

Environmental Precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up

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

Precautions to prevent secondary hazards

Clean contaminated objects and areas thoroughly observing environmental regulations

Reference to Other Sections

Refer to protective measures listed in Sections 8 and 13.

Section 7 - Handling and Storage

Precautions for Safe Handling

Advice on safe handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid

ingestion and inhalation. Avoid dust formation.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

Conditions for Safe Storage, Including any Incompatibilities**Storage Conditions**

Keep refrigerated.

Incompatible Materials

None known.

AS/NZS 2243.10:2004, Safety in laboratories - Storage of chemicals

Section 8 - Exposure Controls and Personal Protection

Control parameters**Exposure limits**

The product does not contain any hazardous materials with occupational exposure limits established.

Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

Appropriate engineering controls**Engineering Measures**

Ensure that eyewash stations and safety showers are close to the workstation location. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

Individual protection measures, such as personal protective equipment**Eye Protection**

Goggles (Australian/New Zealand Standard AS/NZS 1337 - Eye protectors for Industrial applications)

Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	AUS/NZ Standard	Glove comments
Nitrile rubber, Neoprene, Natural rubber, PVC.	See manufacturers recommendations	-	AS/NZS 2161	(minimum requirement)

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Skin and body protection

Long sleeved clothing

Respiratory Protection

Use an AS/NZS 1716 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained in line with AS/NZS 1715 on the use and maintenance of respiratory protective devices

Recommended Filter type:

Particulates filter conforming to EN 143 (or AUS/NZ equivalent)

Recommended half mask:-

Particle filtering: EN149:2001 (or AUS/NZ equivalent)

When RPE is used a face piece Fit Test should be conducted

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls No information available.

Section 9 - Physical and Chemical Properties

Information on basic physical and chemical properties

Physical State	Solid	
Appearance	Light yellow	
Odor	No information available	
Odor Threshold	No data available	
pH	No information available	
Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	No information available	
Flammability (liquid)	Not applicable	Solid
Flammability (solid,gas)	No information available	
Explosion Limits	No data available	
Flash Point	No information available	Method - No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
Viscosity	Not applicable	Solid
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Vapor Pressure	No data available	
Density / Specific Gravity	No data available	
Bulk Density	No data available	
Vapor Density	Not applicable	Solid
Particle characteristics	No data available	

Other information

Molecular Formula	C14 H13 IN2 O2
Molecular Weight	368.17
Evaporation Rate	Not applicable - Solid

Section 10 - Stability and Reactivity

Reactivity	None known, based on information available
Stability	Light sensitive.
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available
Hazardous Polymerization	No information available.
Hazardous Reactions	None under normal processing.
Conditions to Avoid	Heat, flames and sparks.
Incompatible Materials	None known.

Hazardous Decomposition Products Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NO_x). Hydrogen cyanide (hydrocyanic acid). Hydrogen iodide.

Section 11 - Toxicological Information

Acute Effects

Information on likely routes of exposure

Product Information

Inhalation	Not an expected route of exposure.
Eyes	Avoid contact with eyes. Irritating to eyes.
Skin	Avoid contact with skin. May cause irritation. Harmful in contact with skin.
Ingestion	May be harmful if swallowed.

Numerical measures of toxicity

(a) acute toxicity;

Oral	Category 4
Dermal	Category 4
Inhalation	Category 4

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;

Respiratory	No data available
Skin	No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3

Results / Target organs	Respiratory system
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(i) STOT-repeated exposure; No data available

Target Organs	No information available.
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(j) aspiration hazard; Not applicable
Solid

Symptoms / effects, both acute and delayed

No information available.

Section 12 - Ecological Information

Ecotoxicity

Aquatic ecotoxicity	Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.
Terrestrial ecotoxicity	There is no data for this product
Persistence and Degradability	No information available
Bioaccumulative Potential	No information available
Mobility	No information available.

Other adverse effects

Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors
Persistent Organic Pollutant	This product does not contain any known or suspected substance
Ozone Depletion Potential	This product does not contain any known or suspected substance

Section 13 - Disposal Considerations

Waste treatment methods

Waste from Residues/Unused Products	Do not allow into drains or watercourses or dispose of where ground or surface waters may be affected. Wastes, including emptied containers, are controlled wastes and should be disposed of in accordance with all federal, E.P.A., state and local regulations. Assure conformity with all applicable regulations.
Contaminated Packaging	Dispose of this container to hazardous or special waste collection point.
Other Information	Disposal agencies or waste contractors must comply with the New Zealand Hazardous Substances (Disposal) Regulations . Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

Section 14 - Transport Information

NZS 5433:2020

UN-No	UN3439
Proper Shipping Name	NITRILES, SOLID, TOXIC, N.O.S.
Technical Shipping Name	(1-Boc-3-iodoindole-5-carbonitrile)
Hazard Class	6.1
Packing Group	III

IATA

UN-No	UN3439
Proper Shipping Name	NITRILES, SOLID, TOXIC, N.O.S.
Technical Shipping Name	(1-Boc-3-iodoindole-5-carbonitrile)
Hazard Class	6.1

Packing Group III

IMDG/IMO

UN-No UN3439
Proper Shipping Name NITRILES, SOLID, TOXIC, N.O.S.
Technical Shipping Name (1-Boc-3-iodoindole-5-carbonitrile)
Hazard Class 6.1
Packing Group III

Environmental hazards No hazards identified

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code Not applicable, packaged goods

Special Precautions No special precautions required. Please refer to the applicable dangerous goods regulations for additional information.

Additional information None known

Section 15 - Regulatory Information

Safety, health and environmental regulations/legislation specific for the substance or mixture

National Regulations

There are no applicable tolerable exposure limits or environmental exposure limits according to the EPA Controls for Hazardous Substances

Certified handlers, tracking and controlled substance license requirements

Certified handlers are required for some substances. This includes substances requiring a controlled substance license, and most explosives, vertebrates toxic agents, and certain fumigants. Acutely toxic substances which are a Category 1 or 2, such as pesticides also require Certified handlers. Please check the Health and Safety at Work Act 2015 for further information. Tracking is required for some highly hazardous substances. These substances need to be under the control of an appropriately trained person or appropriately secured. Please check the Health and Safety at Work Act 2015 for further information.

Prohibition or notification/licensing requirements

Shown below are details of specific prohibition/notifications or licensing requirements when they apply.

International Regulations

Ozone Depletion Potential This product does not contain any known or suspected substance

Persistent Organic Pollutant This product does not contain any known or suspected substance

Rotterdam Convention (PIC) Not applicable

Authorisation/Restrictions according to EU REACH Not applicable

International Inventories

New Zealand (NZIoC), Australia (AICS), Europe (EINECS/ELINCS/NLP), Korea (KECL), China (IECSC), Taiwan (TCSI), Japan (ENCS), Japan (ISHL), Canada (DSL/NDL), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	NZIoC	AICS	EINECS	ELINCS	NLP	KECL	IECSC	TCSI
1-Boc-3-iodoindole-5-carbonitrile	864685-26-7	-	-	-	-	-	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	PICCS	ISHL	ENCS
1-Boc-3-iodoindole-5-carbonitrile	864685-26-7	-	-	-	-	-	-	-

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

Section 16 - Other Information

This safety data sheet complies with the requirements of the EPA Hazardous Substances (Hazard Classification) Notice 2020 and WorkSafe New Zealand Regulations

Legend

NZIoC - New Zealand Inventory of Chemicals

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

IECSC - Chinese Inventory of Existing Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

NZS 5433:2020 - Transport of Dangerous Goods on Land

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

MARPOL - International Convention for the Prevention of Pollution from Ships

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

WEL - Workplace Exposure Limit

DNEL - Derived No Effect Level

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

VOC - (Volatile Organic Compound)

AICS - Australian Inventory of Chemical Substances

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

ENCS - Japanese Existing and New Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

CAS - Chemical Abstracts Service

ACGIH - American Conference of Governmental Industrial Hygienists

PNEC - Predicted No Effect Concentration

OECD - Organisation for Economic Co-operation and Development

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

ADG - Australian Code for the Transport of Dangerous Goods by Road and Rail

LC50 - Lethal Concentration 50%

ATE - Acute Toxicity Estimate

RPE - Respiratory Protective Equipment

NOEC - No Observed Effect Concentration

BCF - Bioconcentration factor

PBT - Persistent, Bioaccumulative, Toxic

Key literature references and sources for data

HSNO classifications provided in the New Zealand Chemical Classification Information Database (CCID).

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

EPA Guide to classifying hazardous substances in New Zealand

EPA - Assigning a product to an existing HSNO approval guide

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Revision Date

21-Mar-2023

Revision Summary

Not applicable

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of Safety Data Sheet