SAFETY DATA SHEET

according to Regulation UK SI 2019/758 and UK SI 2020/1577 as amended

Creation Date 21-Jun-2010 **Revision Date** 11-Oct-2023 **Revision Number** 7

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product identifier

Product Description: 6-Benzyloxy-1-Boc-indole-2-boronic acid
Cat No. : **430330000; 430330010**
CAS No 850568-66-0
Molecular Formula C20 H22 B N O5

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

Recommended Use Laboratory chemicals.
Uses advised against No Information available

1.3. Details of the supplier of the safety data sheet

Company

UK entity/business name
Fisher Scientific UK
Bishop Meadow Road,
Loughborough, Leicestershire LE11 5RG, United Kingdom

EU entity/business name
Thermo Fisher Scientific
Janssen Pharmaceuticalaan 3a, 2440 Geel, Belgium

E-mail address begel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US:**001-201-796-7100 / **Europe:** +32 14 57 52 99
CHEMTREC Tel. No. **US:**001-800-424-9300 / **Europe:**001-703-527-3887

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

Physical hazards

Based on available data, the classification criteria are not met

Health hazards

Acute oral toxicity	Category 4 (H302)
Skin Corrosion/Irritation	Category 2 (H315)

Serious Eye Damage/Eye Irritation	Category 2 (H319)
Specific target organ toxicity - (single exposure)	Category 3 (H335)

Environmental hazards
Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word **Warning**

Hazard Statements
H302 - Harmful if swallowed
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation

Precautionary Statements
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
P312 - Call a POISON CENTER or doctor if you feel unwell
P280 - Wear protective gloves/protective clothing/eye protection/face protection

2.3. Other hazards

This product does not contain any known or suspected endocrine disruptors

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
6-Benzyloxy-1-Boc-indole-2-boronic acid	850568-66-0		>95	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Acute Tox. 4 (H302)

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

General Advice If symptoms persist, call a physician.

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. Get medical attention.

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

Inhalation Remove to fresh air. If breathing is difficult, give oxygen. Get medical attention.

Self-Protection of the First Aider Use personal protective equipment as required.

4.2. Most important symptoms and effects, both acute and delayed

None reasonably foreseeable.

4.3. Indication of any immediate medical attention and special treatment needed

Notes to Physician Treat symptomatically.

SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media
Water spray, carbon dioxide (CO2), dry chemical, alcohol-resistant foam.

Extinguishing media which must not be used for safety reasons
No information available.

5.2. Special hazards arising from the substance or mixture

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

Hazardous Combustion Products
Burning produces obnoxious and toxic fumes, Carbon monoxide (CO), Carbon dioxide (CO_2), Nitrogen oxides (NOx), Oxides of boron.

5.3. Advice for firefighters

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

6.1. Personal precautions, protective equipment and emergency procedures

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

6.2. Environmental precautions

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

6.3. Methods and material for containment and cleaning up

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

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe handling

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

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

7.2. Conditions for safe storage, including any incompatibilities

Keep refrigerated. To maintain product quality.

Technical Rules for Hazardous Substances (TRGS) 510 Storage Class (LGK) (Germany) Class 11

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

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

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

Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)
No information available

Predicted No Effect Concentration (PNEC)
No information available.

8.2. Exposure controls

Engineering Measures
Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas.
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

Personal protective equipment

Eye Protection Goggles (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber Neoprene Natural rubber PVC	See manufacturers recommendations	-	EN 374	(minimum requirement)

Skin and body protection Long sleeved clothing.

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 compatability, 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.

Respiratory Protection When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.
To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced
Recommended Filter type: Particulates filter conforming to EN 143

Small scale/Laboratory use Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.
Recommended half mask:- Particle filtering: EN149:2001
When RPE is used a face piece Fit Test should be conducted

Environmental exposure controls No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State Solid

Appearance Off-white
Odor No information available
Odor Threshold No data available
Melting Point/Range 102 - 106 °C / 215.6 - 222.8 °F
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	
pH	No information available	
Viscosity	Not applicable	Solid
Water Solubility	Soluble	
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	

9.2. Other information

Molecular Formula	C20 H22 B N O5
Molecular Weight	367.21
Evaporation Rate	Not applicable - Solid

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity

None known, based on information available

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

10.4. Conditions to avoid

Incompatible products. Excess heat. Avoid dust formation.

10.5. Incompatible materials

Strong oxidizing agents. Strong acids.

10.6. Hazardous decomposition products

Burning produces obnoxious and toxic fumes. Carbon monoxide (CO). Carbon dioxide (CO_2). Nitrogen oxides (NOx). Oxides of boron.

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information

(a) acute toxicity;

Oral	Category 4

Dermal	No data available
Inhalation	No data available
(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.
(i) STOT-repeated exposure;	No data available
Target Organs	No information available.
(j) aspiration hazard;	Not applicable Solid
Symptoms / effects,both acute and delayed	No information available.

11.2. Information on other hazards

Endocrine Disrupting Properties	Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

SECTION 12: ECOLOGICAL INFORMATION

12.1. Toxicity

Ecotoxicity effects	Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

12.2. Persistence and degradability

Persistence	Soluble in water, Persistence is unlikely, based on information available.

12.3. Bioaccumulative potential Bioaccumulation is unlikely

12.4. Mobility in soil The product is water soluble, and may spread in water systems Will likely be mobile in the environment due to its water solubility. Highly mobile in soils

12.5. Results of PBT and vPvB assessment No data available for assessment.

12.6. Endocrine disrupting properties
Endocrine Disruptor Information This product does not contain any known or suspected endocrine disruptors

12.7. Other adverse effects
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

13.1. Waste treatment methods

Waste from Residues/Unused Products Dispose of in accordance with the European Directives on waste and hazardous waste. Waste is classified as hazardous. Dispose of in accordance with local regulations.

Contaminated Packaging Dispose of this container to hazardous or special waste collection point.

European Waste Catalogue (EWC) According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

Other Information 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

IMDG/IMO Not regulated

14.1. UN number
14.2. UN proper shipping name
14.3. Transport hazard class(es)
14.4. Packing group

ADR Not regulated

14.1. UN number
14.2. UN proper shipping name
14.3. Transport hazard class(es)
14.4. Packing group

IATA Not regulated

14.1. UN number
14.2. UN proper shipping name
14.3. Transport hazard class(es)

14.4. Packing group

14.5. Environmental hazards No hazards identified

14.6. Special precautions for user No special precautions required.

14.7. Maritime transport in bulk according to IMO instruments Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION

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

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

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
6-Benzyloxy-1-Boc-indole-2-boronic acid	850568-66-0	-	-	-	-	-	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
6-Benzyloxy-1-Boc-indole-2-boronic acid	850568-66-0	-	-	-	-	-	-	-

Legend: X - Listed '-' - Not Listed **KECL** - NIER number or KE number (http://ncis.nier.go.kr/en/main.do)

Authorisation/Restrictions according to EU REACH Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
6-Benzyloxy-1-Boc-indole-2-boronic acid	850568-66-0	-	-	-

Seveso III Directive (2012/18/EC)

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements
6-Benzyloxy-1-Boc-indole-2-boronic acid	850568-66-0	Not applicable	Not applicable

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals
Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?
Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

National Regulations

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

WGK Classification Water endangering class = 3 (self classification)

15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3
H302 - Harmful if swallowed
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation

Legend

CAS - Chemical Abstracts Service

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

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

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

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

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

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

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

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

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Key literature references and sources for data
https://echa.europa.eu/information-on-chemicals
Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

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.

Creation Date	21-Jun-2010
Revision Date	11-Oct-2023
Revision Summary	Not applicable.

This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.

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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