

Creation Date 09-Jul-2010 Revision Date 17-Oct-2014 Revision Number 4

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

1.1. Product identification

Product Description: <u>1H-Indazole-4-boronic acid</u>
Cat No. : <u>430500000; 4305000010</u>

CAS-No 1023595-17-6 **Molecular Formula** C7 H7 B N2 O2

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 Acros Organics BVBA

Janssen Pharmaceuticalaan 3a

2440 Geel, Belgium

E-mail address begel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-ACROS-01 / **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 - Regulation (EC) No 1272/2008

Physical hazards

Based on available data, the classification criteria are not met

Health hazards

Skin Corrosion/irritationCategory 2Serious Eye Damage/Eye IrritationCategory 2Specific target organ toxicity - (single exposure)Category 3

Environmental hazards

Based on available data, the classification criteria are not met

Classification according to EU Directives 67/548/EEC or 1999/45/EC

Symbol(s) Xi - Irritant

R-phrase(s)

R36/37/38 - Irritating to eyes, respiratory system and skin

For the full text of the R-phrases and H-Statements mentioned in this Section, see Section 16.

2.2. Label elements

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Signal Word Warning

Hazard Statements

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

Precautionary Statements

P280 - Wear protective gloves/ protective clothing/ eye protection/ face protection

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water

P304 + P340 - IF INHALED: Remove to fresh air and keep at rest in a position 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/ physician if you feel unwell

2.3. Other hazards

No information available

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

| Component | CAS-No | EC-No. | Weight % | CLP Classification - Regulation (EC) No 1272/2008 | DSD Classification - 67/548/EEC |
|----------------------------|--------------|--------|----------|---|------------------------------------|
| 1H-Indazole-4-boronic acid | 1023595-17-6 | | >95 | Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) STOT SE 3 (H335) | Xi:R36/37/38 |

For the full text of the R-phrases and H-Statements mentioned in this Section, 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.

Obtain medical attention.

Skin Contact Wash off immediately with plenty of water for at least 15 minutes. Get medical attention if

symptoms occur.

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

symptoms occur.

Inhalation Move to fresh air. If breathing is difficult, give oxygen. Get medical attention immediately if

symptoms occur.

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Protection of First-aidersUse personal protective equipment.

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

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

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

Carbon monoxide (CO), Carbon dioxide (CO2), 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. Avoid dust formation.

6.2. Environmental precautions

Should not be released into the environment.

6.3. Methods and material for containment and cleaning up

Sweep up or vacuum up spillage and collect in suitable container 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. Ensure adequate ventilation. Avoid dust formation. Do not get in eyes, on skin, or on 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.

To maintain product quality. Protect from moisture.

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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.

Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents.

MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

Derived No Effect Level (DNEL) No information available

| Route of exposure | Acute effects (local) | Acute effects (systemic) | Chronic effects (local) | Chronic effects (systemic) |
|-------------------|-----------------------|--------------------------|----------------------------|----------------------------|
| Oral | | | | |
| Dermal | | | | |
| Inhalation | | | | |

Predicted No Effect Concentration No information available. **(PNEC)**

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

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Nitrile rubber See manufacturers - EN 374 (minimum requirement)
Neoprene recommendations

Natural rubber PVC

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

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

Environmental exposure controls No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

AppearanceWhite - TanPhysical StateSolid

Odor No information available
Odor Threshold No data available

pH No information available

Melting Point/Range 166 - 168 °C / 330.8 - 334.4 °F Measured

Softening Point No data available

Boiling Point/Range No information available

Flash Point No information available Method - No information available

Evaporation Rate Not applicable Solid

Flammability (solid,gas) No information available

Explosion Limits No data available

Vapor Pressure
No data available
Vapor Density
Not applicable

Specific Gravity / Density No data available Bulk Density No data available

Water Solubility Insoluble

Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

Autoignition Temperature

Not applicable

No data available

Viscosity Not applicable Solid

ACR43050

Solid

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Explosive Properties No information available Oxidizing Properties No information available

9.2. Other information

Molecular Formula C7 H7 B N2 O2

Molecular Weight 161.96

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

Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NOx). Oxides of boron.

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on toxicological effects

Product Information No acute toxicity information is available for this product

(a) acute toxicity;

Oral No data available
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

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(i) STOT-repeated exposure; No data available

Target Organs Skin, Respiratory system, Eyes.

(j) aspiration hazard; Not applicable

Solid

Symptoms / effects,both acute and No information available

delayed

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 Insoluble in water.

12.3. Bioaccumulative potential May have some potential to bioaccumulate

12.4. Mobility in soil Spillage unlikely to penetrate soil Is not likely mobile in the environment due its low water

solubility.

12.5. Results of PBT and vPvB

assessment

No data available for assessment.

12.6. Other adverse effects

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

This product does not contain any known or suspected substance 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 Catalogue, 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

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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. Transport in bulk according to Not applicable, packaged goods

Annex II of MARPOL73/78 and the

IBC Code

SECTION 15: REGULATORY INFORMATION

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

International Inventories X = listed The product is classified and labeled according to EC directives or corresponding

national laws The product is classified and labeled in accordance with Directive 1999/45/EC

National Regulations

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

Take note of Dir 94/33/EC on the protection of young people at work

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

15.2. Chemical safety assessment

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

SECTION 16: OTHER INFORMATION

Full text of R-phrases referred to under sections 2 and 3

R36/37/38 - Irritating to eyes, respiratory system and skin

Full text of H-Statements referred to under sections 2 and 3

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

Legend

CAS - Chemical Abstracts Service TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

EINECS/ELINCS - European Inventory of Existing Commercial Chemical DSL/NDSL - Canadian Domestic Substances List/Non-Domestic 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

Substances List

ENCS - Japanese Existing and New Chemical Substances AICS - Australian Inventory of Chemical Substances NZIoC - New Zealand Inventory of Chemicals

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WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment
LC50 - Lethal Concentration 50%
NOFC - No Observed Effect Concentration

NOEC - No Observed Effect Concentration **PBT** - Persistent, Bioaccumulative, Toxic

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

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

PNEC - Predicted No Effect Concentration

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%
POW - Partition coefficient Octanol:Water

VPVB - very Persistent, very Bioaccumulative

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

 $\mbox{\bf MARPOL}$ - International Convention for the Prevention of Pollution from

Ships

ATE - Acute Toxicity Estimate

VOC - Volatile Organic Compounds

Key literature references and sources for data

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 Date09-Jul-2010Revision Date17-Oct-2014

Revision Summary Update to Format, (M)SDS sections updated, 2, 3, 4, 5, 7, 8, 9, 11, 12.

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

Disclaimer

The information provided on 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 guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as 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 material or in any process, unless specified in the text.

End of Safety Data Sheet