

Revision Date 16-Oct-2014

Revision Number 4

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

### 1.1. Product identification

**Product Description:** 4-Chloro-3-cyanophenylboronic acid  
**Cat No. :** 430420000; 430420010; 430420050  
**CAS-No** 871332-95-5  
**Molecular Formula** C7 H5 B Cl N 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 Pharmaceuticaaan 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

Acute oral toxicity	Category 4
Acute dermal toxicity	Category 4
Acute Inhalation Toxicity - Dusts and Mists	Category 4

#### 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)** Xn - Harmful  
**R-phrases(s)** R20/21/22 - Harmful by inhalation, in contact with skin and if swallowed

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

H302 - Harmful if swallowed  
H312 - Harmful in contact with skin  
H332 - Harmful if inhaled

## Precautionary Statements

P280 - Wear protective gloves/ protective clothing  
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
4-Chloro-3-cyanophenylboronic acid	871332-95-5		>=95	Acute Tox. 4 (H302) Acute Tox. 4 (H312) Acute Tox. 4 (H332)	Xn;R20/21/22

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. Obtain medical attention.

#### 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-aiders** Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

## **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 (CO<sub>2</sub>), Oxides of boron, Nitrogen oxides (NO<sub>x</sub>), Hydrogen chloride gas.

### **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. See Section 12 for additional ecological information.

### **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. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Avoid dust formation.

### **7.2. Conditions for safe storage, including any incompatibilities**

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Keep container tightly closed in a dry and well-ventilated place.  
To maintain product quality. Keep refrigerated.

## 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

<u>Route of exposure</u>	<u>Acute effects (local)</u>	<u>Acute effects (systemic)</u>	<u>Chronic effects (local)</u>	<u>Chronic effects (systemic)</u>
Oral Dermal Inhalation				

**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** Safety glasses with side-shields (European standard - EN 166)

**Hand Protection** Protective gloves

<u>Glove material</u>	<u>Breakthrough time</u>	<u>Glove thickness</u>	<u>EU standard</u>	<u>Glove comments</u>
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Nitrile rubber Neoprene Natural rubber PVC	See manufacturers recommendations	-	EN 374	(minimum requirement)
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**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 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.

**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

<b>Appearance</b>	Pale yellow	
<b>Physical State</b>	Solid	
<b>Odor</b>	No information available	
<b>Odor Threshold</b>	No data available	
<b>pH</b>	No information available	
<b>Melting Point/Range</b>	300 - 304 °C / 572 - 579.2 °F	Based on available literature
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	No information available	
<b>Flash Point</b>	No information available	<b>Method -</b> No information available
<b>Evaporation Rate</b>	Not applicable	Solid
<b>Flammability (solid,gas)</b>	No information available	
<b>Explosion Limits</b>	No data available	
<b>Vapor Pressure</b>	No data available	
<b>Vapor Density</b>	Not applicable	Solid
<b>Specific Gravity / Density</b>	No data available	
<b>Bulk Density</b>	No data available	
<b>Water Solubility</b>	No information available	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Autoignition Temperature</b>	Not applicable	
<b>Decomposition Temperature</b>	No data available	
<b>Viscosity</b>	Not applicable	Solid

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**Explosive Properties** No information available  
**Oxidizing Properties** No information available

## 9.2. Other information

**Molecular Formula** C7 H5 B Cl N O2  
**Molecular Weight** 181.39

## 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 (CO<sub>2</sub>). Oxides of boron. Nitrogen oxides (NO<sub>x</sub>). Hydrogen chloride gas.

## SECTION 11: TOXICOLOGICAL INFORMATION

### 11.1. Information on toxicological effects

#### Product Information

(a) acute toxicity;  
Oral Category 4  
Dermal Category 4  
Inhalation Category 4

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

(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

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(h) STOT-single exposure;	No data available
(i) STOT-repeated exposure;	No data available
Target Organs	Skin, Respiratory system, Eyes.
(j) aspiration hazard;	Not applicable Solid
Symptoms / effects,both acute and delayed	No information available

## SECTION 12: ECOLOGICAL INFORMATION

<u>12.1. Toxicity</u> Ecotoxicity effects	Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.
<u>12.2. Persistence and degradability</u>	No information available
<u>12.3. Bioaccumulative potential</u>	No information available
<u>12.4. Mobility in soil</u>	No information available
<u>12.5. Results of PBT and vPvB assessment</u>	No data available for assessment.
<u>12.6. Other adverse effects</u> 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

<u>13.1. Waste treatment methods</u>	
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

<u>IMDG/IMO</u>	Not regulated
<u>14.1. UN number</u>	
<u>14.2. UN proper shipping name</u>	
<u>14.3. Transport hazard class(es)</u>	
<u>14.4. Packing group</u>	
<u>ADR</u>	Not regulated

14.1. UN number

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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 Annex II of MARPOL73/78 and the IBC Code Not applicable, packaged goods

## 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 work

### 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

R20/21/22 - Harmful by inhalation, in contact with skin and if swallowed

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

H302 - Harmful if swallowed  
H312 - Harmful in contact with skin  
H332 - Harmful if inhaled

### 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/NDL** - 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



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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%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**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

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

**IMO/MDG** - 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 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.

**Revision Date** 16-Oct-2014

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

**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**