

Creation Date 16-Jun-2010 Revision Date 12-Jan-2015 Revision Number 4

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

#### 1.1. Product identification

Product Description: 3-Cyano-5-fluorophenylboronic acid

Cat No.: 430460000; 430460010

**CAS-No** 304858-67-1 **Molecular Formula** C7 H5 B F 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 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**

Acute oral toxicityCategory 4Skin 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) Xn - Harmful

R-phrase(s) R22 - Harmful if swallowed

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



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**

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
3-Cyano-5-fluorophenylboronic acid	304858-67-1		>95	Acute Tox. 4 (H302) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) STOT SE 3 (H335)	Xn;R22 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

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. Obtain medical attention. Get medical

attention immediately if symptoms occur.

#### 3-Cyano-5-fluorophenylboronic acid

**Protection of First-aiders** 

Ensure that medical personnel are aware of the material(s) involved, take precautions to

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protect themselves and prevent spread of contamination.

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

No information available.

#### 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. Keep product and empty container away from heat and sources of ignition.

#### **Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Nitrogen oxides (NOx), Hydrogen fluoride, 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

Use personal protective equipment. Ensure adequate ventilation. Avoid dust formation. Avoid contact with skin, eyes and clothing.

#### 6.2. Environmental precautions

Avoid release to 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. Avoid dust formation.

#### 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

#### 3-Cyano-5-fluorophenylboronic acid

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			
Route of exposure	Acute effects (local)	Acute effects	Chronic effects	Chronic effects
		(systemic)	(local)	(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 Nitrile rubber Neoprene Natural rubber PVC	Breakthrough time See manufacturers recommendations	Glove thickness	<b>EU standard</b> EN 374	Glove comments (minimum requirement)
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**Skin and body protection**Wear appropriate protective gloves and clothing to prevent skin exposure

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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

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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 Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure Small scale/Laboratory use

Solid

Solid

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

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

**Environmental exposure controls** No information available.

## **SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES**

#### 9.1. Information on basic physical and chemical properties

White **Appearance Physical State** Solid

Odor No information available **Odor Threshold** No data available No information available Hq **Melting Point/Range** No data available

**Softening Point** No data available **Boiling Point/Range** No information available Flash Point No data available

Method - No information available Not applicable **Evaporation Rate** Solid

Flammability (solid,gas) No information available

**Explosion Limits** No data available

**Vapor Pressure** No data available Not applicable **Vapor Density** 

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

Water Solubility No information available Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

**Autoignition Temperature** Not applicable **Decomposition Temperature** No data available **Viscosity** Not applicable

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

9.2. Other information

C7 H5 B F N O2 Molecular Formula

**Molecular Weight** 164.93

## **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). Hydrogen fluoride.

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Oxides of boron.

## **SECTION 11: TOXICOLOGICAL INFORMATION**

#### 11.1. Information on toxicological effects

#### **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

(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

3-Cyano-5-fluorophenylboronic acid

deland

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 No information available

12.3. Bioaccumulative potential No information available

**12.4. Mobility in soil** No information available

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

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

14.4. Packing group

<u>IATA</u> 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

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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

X = listed**International Inventories** 

#### **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

R22 - Harmful if swallowed

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

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

H302 - Harmful if swallowed

H315 - Causes skin irritation

H319 - Causes serious eve irritation

H335 - May cause respiratory irritation

#### Legend

**CAS** - Chemical Abstracts Service

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

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

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

Key literature references and sources for data

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

Substances List

**ENCS** - Japanese Existing and New Chemical Substances AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

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

MARPOL - International Convention for the Prevention of Pollution from

ATE - Acute Toxicity Estimate

VOC - Volatile Organic Compounds

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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.

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Revision Summary Update to Format.

## 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**