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**Revision Number** 4

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

1.1. Product identification

 Product Description:
 5-Cyano-2-fluorophenylboronic acid

 Cat No. :
 430230000; 430230010; 430230050

 CAS-No
 468718-30-1

 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

CompanyAcros Organics BVBAJanssen Pharmaceuticalaan 3a2440 Geel, BelgiumE-mail addressbegel.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

Health hazards	
Acute oral toxicity	Category 4
Skin Corrosion/irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
	Category 3
Serious Eye Damage/Eye Irritation Specific target organ toxicity - (single exposure)	Category 2

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

### 5-Cyano-2-fluorophenylboronic acid



### Signal Word

Warning

### Hazard Statements

H335 - May cause respiratory irritation

H302 - Harmful if swallowed

H319 - Causes serious eye irritation

H315 - Causes skin 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
5-Cyano-2-fluorophenylboronic acid	468718-30-1		>95	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Acute Tox. 4 (H302)	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. Get medical attention immediately if symptoms occur. If breathing is difficult, give oxygen.

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

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

5-Cyano-2-fluorophenylboronic acid

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

Burning produces obnoxious and toxic fumes, Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Oxides of boron, Hydrogen halides, Nitrogen oxides (NOx).

### 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. 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. Avoid dust formation. Do not breathe dust. Do not get in eyes, on skin, or on clothing.

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

Keep container tightly closed in a dry and well-ventilated place. 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 (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 equip Eye Protection	nent Goggles (European standard - EN 166	)
Hand Protection	Protective gloves	
Glove material Brea	akthrough time Glove thickness EU stand	ard Glove comments

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

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure

Inspect gloves before use.

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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 <b>Recommended Filter type:</b> 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. <b>Recommended half mask:-</b> 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

Appearance Physical State	White Solid	
Odor Odor Threshold pH Melting Point/Range Softening Point Boiling Point/Range	No information available No data available No information available 350 - 353 °C / 662 - 667.4 °F No data available No information available	Measured
Flash Point Evaporation Rate Flammability (solid,gas) Explosion Limits	No data available Not applicable No information available No data available	<b>Method -</b> No information available Solid
Vapor Pressure Vapor Density Specific Gravity / Density Bulk Density Water Solubility Solubility in other solvents Partition Coefficient (n-octanol/wate	•	Solid
Autoignition Temperature Decomposition Temperature Viscosity	Not applicable No data available Not applicable	Solid

Explosive Properties	No information available	
Oxidizing Properties	No information available	
9.2. Other information		
Molecular Formula	C7 H5 B F N O2	
Molecular Weight	164.93	
	SECTION 10: STABILITY AND REACTIVITY	
10.1. Reactivity		
<u>ion Rodonny</u>	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 r	products	

### 10.6. Hazardous decomposition products

5-Cyano-2-fluorophenylboronic acid

Burning produces obnoxious and toxic fumes. Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Oxides of boron. Hydrogen halides. Nitrogen oxides (NOx).

# **SECTION 11: TOXICOLOGICAL INFORMATION**

### 11.1. Information on toxicological effects

### **Product Information**

(a) acute toxicity; Oral Dermal Inhalation	Category 4 No data available No data available
(b) skin corrosion/irritation;	Category 2
(c) serious eye damage/irritation;	Category 2
(d) respiratory or skin sensitization Respiratory Skin	; No data available 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 delayed

5-Cyano-2-fluorophenylboronic acid

### **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.
12.2. Persistence and degradability	No information available
12.3. Bioaccumulative potential	No information available
<u>12.4. Mobility in soil</u>	No information available
12.5. Results of PBT and vPvB assessment	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**

### 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

ACR43023

5-Cyano-2-fluorophenylboronic acid

### 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

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

### **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 eye irritation

H335 - May cause respiratory irritation

#### Legend

oxic Substances Control Act Section 8(b)
Domestic Substances List/Non-Domestic
ng and New Chemical Substances
ory of Chemical Substances ventory of Chemicals

### 5-Cyano-2-fluorophenylboronic acid

WEL - Workplace Exposure Limit	TWA - Time Weighted Average
ACGIH - American Conference of Governmental Industrial Hygienists	IARC - International Agency for Research on Cancer
DNEL - Derived No Effect Level	PNEC - Predicted No Effect Concentration
RPE - Respiratory Protective Equipment	LD50 - Lethal Dose 50%
LC50 - Lethal Concentration 50%	EC50 - Effective Concentration 50%
NOEC - No Observed Effect Concentration	POW - Partition coefficient Octanol:Water
PBT - Persistent, Bioaccumulative, Toxic	vPvB - very Persistent, very Bioaccumulative
<ul> <li>ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road</li> <li>IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code</li> <li>OECD - Organisation for Economic Co-operation and Development BCF - Bioconcentration factor</li> </ul>	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.

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Revision Summary	Not applicable.

### 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