

Creation Date 30-Jan-2015

Revision Date 05-Feb-2015

Revision Number 2

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

1.1. Product identification

Product Description: **7-Azaindole-5-boronic acid, pinacol ester, 97%**
 Cat No. : **455850000; 455850010; 455852500**
 CAS-No **754214-56-7**
 Molecular Formula **C₁₃H₁₇BN₂O₂**

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
Skin Corrosion/irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific 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-phrases 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

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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 to fresh air and keep at rest in a position comfortable for breathing
- P312 - Call a POISON CENTER or doctor/ physician if you feel unwell
- P280 - Wear protective gloves/ protective clothing/ eye protection/ face protection

2.3. Other hazards

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.2. Mixtures

Component	CAS-No	EC-No.	Weight %	CLP Classification - Regulation (EC) No 1272/2008	DSD Classification - 67/548/EEC
7-Azaindole-5-boronic acid, pinacol ester	754214-56-7		>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

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. Obtain medical attention.

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Protection of First-aiders Use 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).

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.

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. 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

Keep containers tightly closed in a dry, cool and well-ventilated place.

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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 (PNEC) No information available.

8.2. Exposure controls

Engineering Measures

Ensure that eyewash stations and safety showers are close to the workstation location.

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	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)

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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

Appearance	Off-white	
Physical State	Solid	
Odor	No information available	
Odor Threshold	No data available	
pH	Not applicable	
Melting Point/Range	244 - 246 °C / 471.2 - 474.8 °F	Measured
Softening Point	No data available	
Boiling Point/Range	Not applicable	
Flash Point	Not applicable	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	Solid
Specific Gravity / Density	No data available	
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	Solid
Explosive Properties	No information available	
Oxidizing Properties	No information available	

9.2. Other information

Molecular Formula	C13H17BN2O2
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SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity

None known, based on information available

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10.2. Chemical stability

Stable under normal conditions

10.3. Possibility of hazardous reactions

Hazardous Polymerization Hazardous Reactions

Hazardous polymerization does not occur.
None under normal processing.

10.4. Conditions to avoid

Incompatible products. Excess heat. Avoid dust formation.

10.5. Incompatible materials

Acids. Oxidizing agents.

10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO₂).

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

Toxicology data for the components

(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 No information available.

(j) aspiration hazard; Not applicable
Solid

Symptoms / effects, both acute and delayed No information available

SECTION 12: ECOLOGICAL INFORMATION

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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

This product does not contain any known or suspected endocrine disruptors

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

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. 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

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

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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 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

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

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

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

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

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 Ships

ATE - Acute Toxicity Estimate

VOC - Volatile Organic Compounds

Classification and procedure used to derive the classification for mixtures according to Regulation (EC) 1272/2008 [CLP]:

ACR45585

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Physical hazards	On basis of test data
Health Hazards	Calculation method
Environmental hazards	Calculation method

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	30-Jan-2015
Revision Date	05-Feb-2015
Revision Summary	(M)SDS sections updated, 15.

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