

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING**1.1. Product identifier**

Product Description: 3-(Cyanomethyl)benzeneboronic acid pinacol ester
Cat No. : H52618
CAS No 396131-82-1
Molecular Formula C14 H18 B N O2
REACH registration number -

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**

Avocado Research Chemicals Ltd.
(Part of Thermo Fisher Scientific)
Shore Road, Heysham
Lancashire, LA3 2XY,
United Kingdom
Office Tel: +44 (0) 1524 850506
Office Fax: +44 (0) 1524 850608

E-mail address begel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **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 - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567****Physical hazards**

Based on available data, the classification criteria are not met

Health hazards

Acute oral toxicity

Category 4 (H302)

SAFETY DATA SHEET

3-(Cyanomethyl)benzeneboronic acid pinacol ester

Revision Date 04-Feb-2024

Skin Corrosion/Irritation
Serious Eye Damage/Eye Irritation
Specific target organ toxicity - (single exposure)

Category 2 (H315)
Category 2 (H319)
Category 3 (H335)

Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: 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

P301 + P330 + P331 - IF SWALLOWED: rinse mouth. Do NOT induce vomiting
P312 - Call a POISON CENTER or doctor if you feel unwell
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P337 + P313 - If eye irritation persists: Get medical advice/attention
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
P280 - Wear protective gloves/protective clothing/eye protection/face protection
P332 + P313 - If skin irritation occurs: Get medical advice/attention

2.3. Other hazards

This product does not contain any known or suspected endocrine disruptors

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

| Component | CAS No | EC No | Weight % | CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567 |
|---|-------------|-------|----------|---|
| 3-(Cyanomethyl)phenylboronic acid pinacol ester | 396131-82-1 | | >95 | Acute Tox. 4 (H302) Eye Irrit. 2 (H319) STOT SE 3 (H335) Skin Irrit. 2 (H315) |

REACH registration number

-

Full text of Hazard Statements: see section 16

SAFETY DATA SHEET

3-(Cyanomethyl)benzeneboronic acid pinacol ester

Revision Date 04-Feb-2024

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. Get medical attention. |
| Skin Contact | Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician. |
| Ingestion | Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur. |
| Inhalation | Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur. |
| Self-Protection of the First Aider | 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

Water spray, carbon dioxide (CO₂), dry chemical, alcohol-resistant foam.

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

Thermal decomposition can lead to release of irritating gases and vapors, Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x), 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 as required. Avoid dust formation.

6.2. Environmental precautions

SAFETY DATA SHEET

3-(Cyanomethyl)benzeneboronic acid pinacol ester

Revision Date 04-Feb-2024

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 and shovel into suitable containers 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/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Avoid dust formation.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

7.2. Conditions for safe storage, including any incompatibilities

Keep containers tightly closed in a dry, cool and well-ventilated place. Store under an inert atmosphere. Protect from moisture.

Technical Rules for Hazardous Substances (TRGS) 510 Class 11
Storage Class (LGK) (Germany)

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

Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

No information available

Predicted No Effect Concentration (PNEC)

No information available.

SAFETY DATA SHEET

3-(Cyanomethyl)benzeneboronic acid pinacol ester

Revision Date 04-Feb-2024

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

No protective equipment is needed under normal use conditions.

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

Small scale/Laboratory use

Maintain adequate ventilation

Environmental exposure controls

No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

| | | |
|---------------------------|-----------------------------------|--|
| Physical State | Solid | |
| Appearance | Orange | |
| Odor | No information available | |
| Odor Threshold | No data available | |
| Melting Point/Range | 61 - 63 °C / 141.8 - 145.4 °F | |
| Softening Point | No data available | |
| Boiling Point/Range | No information available | |
| Flammability (liquid) | Not applicable | |
| Flammability (solid,gas) | No information available | |
| Explosion Limits | No data available | |
| Flash Point | No information available | |
| Autoignition Temperature | No data available | |
| Decomposition Temperature | No data available | |
| pH | No information available | |
| Viscosity | Not applicable | |
| Water Solubility | Solid | |
| | Method - No information available | |

SAFETY DATA SHEET

3-(Cyanomethyl)benzeneboronic acid pinacol ester

Revision Date 04-Feb-2024

| | |
|--|----------------------------|
| Solubility in other solvents | No information available |
| Partition Coefficient (n-octanol/water) | No data available |
| Vapor Pressure | No data available |
| Density / Specific Gravity | No data available |
| Bulk Density | No data available |
| Vapor Density | Not applicable |
| Particle characteristics | Solid No data available |

9.2. Other information

| | |
|--------------------------|------------------------|
| Molecular Formula | C14 H18 B N O2 |
| Molecular Weight | 243.12 |
| Evaporation Rate | Not applicable - Solid |

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity

None known, based on information available

10.2. Chemical stability

Stable under recommended storage 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. Protect from moisture.

10.5. Incompatible materials

Strong oxidizing agents. Strong acids. Strong bases.

10.6. Hazardous decomposition products

Thermal decomposition can lead to release of irritating gases and vapors. Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NO_x). Oxides of boron.

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

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 |

SAFETY DATA SHEET

3-(Cyanomethyl)benzeneboronic acid pinacol ester

Revision Date 04-Feb-2024

| | |
|------------------------------------|---|
| (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 Results / Target organs Respiratory system. |
| (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. |

11.2. Information on other hazards

| | |
|--|---|
| Endocrine Disrupting Properties | Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors. |
|--|---|

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. Endocrine disrupting properties

Endocrine Disruptor Information This product does not contain any known or suspected endocrine disruptors

12.7. Other adverse effects

Persistent Organic Pollutant Ozone Depletion Potential This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

SAFETY DATA SHEET

3-(Cyanomethyl)benzeneboronic acid pinacol ester

Revision Date 04-Feb-2024

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 Catalog, 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

14.6. Special precautions for user No special precautions required.

14.7. Maritime transport in bulk according to IMO instruments Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION

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

International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCS), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

SAFETY DATA SHEET

3-(Cyanomethyl)benzeneboronic acid pinacol ester

Revision Date 04-Feb-2024

| Component | CAS No | TSCA | TSCA Inventory notification - Active-Inactive | DSL | NDSL | AICS | NZIoC | PICCS |
|---|-------------|------|---|-----|------|------|-------|-------|
| 3-(Cyanomethyl)phenylboronic acid pinacol ester | 396131-82-1 | - | - | - | - | - | - | - |

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

Authorisation/Restrictions according to EU REACH

Not applicable

| Component | CAS No | REACH (1907/2006) - Annex XIV - Substances Subject to Authorization | REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances | REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC) |
|---|-------------|---|---|---|
| 3-(Cyanomethyl)phenylboronic acid pinacol ester | 396131-82-1 | - | - | - |

Seveso III Directive (2012/18/EC)

| Component | CAS No | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements |
|---|-------------|---|--|
| 3-(Cyanomethyl)phenylboronic acid pinacol ester | 396131-82-1 | Not applicable | Not applicable |

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

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 .

National Regulations

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

WGK Classification Water endangering class = 3 (self classification)

15.2. Chemical safety assessment

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

SECTION 16: OTHER INFORMATION

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

H302 - Harmful if swallowed

H315 - Causes skin irritation

SAFETY DATA SHEET

3-(Cyanomethyl)benzeneboronic acid pinacol ester

Revision Date 04-Feb-2024

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

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

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 Predicted No Effect Concentration (PNEC)

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/IMDG - 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 Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

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.

Prepared By

Health, Safety and Environmental Department

Creation Date

15-Nov-2011

Revision Date

04-Feb-2024

Revision Summary

New emergency telephone response service provider.

This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.

Disclaimer

The information provided in 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 guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered 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 materials or in any process, unless specified in the text

End of Safety Data Sheet