SAFETY DATA SHEET

2-(TRIFLUOROMETHYL)PYRIDINE-4-BORONIC ACID, PINACOL ESTER

Compilation date: 29/05/2013

Revision No: 1

Section 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

Product name: 2-(TRIFLUOROMETHYL)PYRIDINE-4-BORONIC ACID, PINACOL ESTER

CAS number: 1036990-42-7

Product code: PC49307

Synonyms: 4-(4,4,5,5-TETRAMETHYL-1,3,2-DIOXABOROLAN-2-YL)-2-(TRIFLUOROMETHYL)PYRIDINE

4,4,5,5-TETRAMETHYL-2-[2-(TRIFLUOROMETHYL)PYRIDIN-4-YL]-1,3,2-DIOXABOROLANE

1.2. Relevant identified uses of the substance or mixture and uses advised against

1.3. Details of the supplier of the safety data sheet

Company name: Apollo Scientific Ltd

Units 3 & 4

Parkway

Denton

Manchester

M34 3SG

UK

Tel: 0161 337 9971

Fax: 0161 336 6932

Email: david.tideswell@apolloscientific.co.uk

1.4. Emergency telephone number

Section 2: Hazards identification

2.1. Classification of the substance or mixture

Classification under CHIP: Xn: R20/21/22; Xi: R36/37/38

Classification under CLP: Acute Tox. 4: H302+312+332; STOT SE 3: H335; Eye Irrit. 2: H319; Skin Irrit. 2: H315

Most important adverse effects: Harmful by inhalation, in contact with skin and if swallowed. Irritating to eyes, respiratory system and skin.

2.2. Label elements

Label elements under CLP:

Hazard statements: H302+312+332: Harmful if swallowed, in contact with skin or if inhaled.

H315: Causes skin irritation.

H319: Causes serious eye irritation.

H335: May cause respiratory irritation.

Signal words: Warning

Hazard pictograms: GHS07: Exclamation mark

[cont...]

Precautionary statements: P280: Wear protective gloves/protective clothing/eye protection/face protection.

Label elements under CHIP:

Hazard symbols: Harmful.

Risk phrases: R20/21/22: Harmful by inhalation, in contact with skin and if swallowed.

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

2.3. Other hazards

PBT: This substance is not identified as a PBT substance.

Section 3: Composition/information on ingredients

3.1. Substances

Chemical identity: 2-(TRIFLUOROMETHYL)PYRIDINE-4-BORONIC ACID, PINACOL ESTER

Section 4: First aid measures

4.1. Description of first aid measures

Skin contact: Remove all contaminated clothes and footwear immediately unless stuck to skin. Drench the affected skin with running water for 10 minutes or longer if substance is still on skin. Consult a doctor.

Eye contact: Bathe the eye with running water for 15 minutes. Consult a doctor.

Ingestion: Wash out mouth with water. Do not induce vomiting. If conscious, give half a litre of water to drink immediately. Consult a doctor.

Inhalation: Remove casualty from exposure ensuring one's own safety whilst doing so. Consult a doctor.

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

Skin contact: There may be irritation and redness at the site of contact.

Eye contact: There may be irritation and redness. The eyes may water profusely.

Ingestion: There may be soreness and redness of the mouth and throat. Nausea and stomach pain may occur. There may be vomiting.

Inhalation: There may be irritation of the throat with a feeling of tightness in the chest.

4.3. Indication of any immediate medical attention and special treatment needed

Section 5: Fire-fighting measures

5.1. Extinguishing media

Extinguishing media: Carbon dioxide, dry chemical powder, foam. Suitable extinguishing media for the surrounding fire should be used.

[cont...]

5.2. Special hazards arising from the substance or mixture

Exposure hazards: In combustion emits toxic fumes. Carbon oxides. Nitrogen oxides (NOx). Hydrogen fluoride (HF). Borane/boron oxides.

5.3. Advice for fire-fighters

Advice for fire-fighters: Wear self-contained breathing apparatus. Wear protective clothing to prevent contact with skin and eyes.

Section 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions: Refer to section 8 of SDS for personal protection details. If outside do not approach from downwind. If outside keep bystanders upwind and away from danger point. Mark out the contaminated area with signs and prevent access to unauthorised personnel.

6.2. Environmental precautions

Environmental precautions: Do not discharge into drains or rivers.

6.3. Methods and material for containment and cleaning up

Clean-up procedures: Transfer to a closable, labelled salvage container for disposal by an appropriate method.

6.4. Reference to other sections

Section 7: Handling and storage

7.1. Precautions for safe handling

Handling requirements: Avoid direct contact with the substance. Ensure there is sufficient ventilation of the area. Do not handle in a confined space. Avoid the formation or spread of dust in the air. Only use in fume hood.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions: Store in cool, well ventilated area. Keep container tightly closed. Store under Argon.

Suitable packaging: Must only be kept in original packaging.

7.3. Specific end use(s)

Specific end use(s): No data available.

Section 8: Exposure controls/personal protection

8.1. Control parameters

Workplace exposure limits: No data available.

8.2. Exposure controls

Engineering measures: Ensure there is sufficient ventilation of the area.

Respiratory protection: Self-contained breathing apparatus must be available in case of emergency. Respiratory protective device with particle filter.

[cont...]

Hand protection: Protective gloves.

Eye protection: Safety glasses. Ensure eye bath is to hand.

Skin protection: Protective clothing.

Section 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

State: Solid

9.2. Other information

Other information: No data available.

Section 10: Stability and reactivity

10.1. Reactivity

Reactivity: Stable under recommended transport or storage conditions.

10.2. Chemical stability

Chemical stability: Stable under normal conditions.

10.3. Possibility of hazardous reactions

Hazardous reactions: Hazardous reactions will not occur under normal transport or storage conditions.

10.4. Conditions to avoid

Conditions to avoid: Heat.

10.5. Incompatible materials

Materials to avoid: Strong oxidising agents. Strong acids.

10.6. Hazardous decomposition products

Haz. decomp. products: In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen oxides (NOx). Boron Oxides Hydrogen fluoride (HF).

Section 11: Toxicological information

11.1. Information on toxicological effects

Relevant hazards for substance:

Hazard	Route	Basis
Acute toxicity (ac. tox. 4)	INH DRM ING	Based on test data
Skin corrosion/irritation	DRM	Based on test data
Serious eye damage/irritation	OPT	Based on test data
STOT-single exposure	INH	Based on test data

Symptoms / routes of exposure

Skin contact: There may be irritation and redness at the site of contact.

Eye contact: There may be irritation and redness. The eyes may water profusely.

[cont...]

Ingestion: There may be soreness and redness of the mouth and throat. Nausea and stomach pain may occur. There may be vomiting.

Inhalation: There may be irritation of the throat with a feeling of tightness in the chest.

Other information: High hazard Class III chemical : assigned according to Cramer decision tree with extensions (predicted *)

Section 12: Ecological information

12.1. Toxicity

Ecotoxicity values: No data available.

12.2. Persistence and degradability

Persistence and degradability: Persistent chemical (predicted *)

12.3. Bioaccumulative potential

Bioaccumulative potential: No data available.

12.4. Mobility in soil

Mobility: No data available.

12.5. Results of PBT and vPvB assessment

PBT identification: This substance is not identified as a PBT substance.

12.6. Other adverse effects

Other adverse effects: No data available.

Section 13: Disposal considerations

13.1. Waste treatment methods

Disposal operations: MATERIAL SHOULD BE DISPOSED OF IN ACCORDANCE WITH LOCAL, STATE AND FEDERAL REGULATIONS

Disposal of packaging: Dispose of as special waste in compliance with local and national regulations Observe all federal, state and local environmental regulations.

NB: The user's attention is drawn to the possible existence of regional or national regulations regarding disposal.

Section 14: Transport information

14.1. UN number

UN number: UNnone

14.2. UN proper shipping name

Shipping name: NOT CLASSIFIED AS DANGEROUS IN THE MEANING OF TRANSPORT REGULATIONS.

14.3. Transport hazard class(es)

[cont...]

14.4. Packing group

14.5. Environmental hazards

Environmentally hazardous: No **Marine pollutant:** No

14.6. Special precautions for user

Section 15: Regulatory information

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

15.2. Chemical Safety Assessment

Chemical safety assessment: A chemical safety assessment has not been carried out for the substance or the mixture by the supplier.

Section 16: Other information

Other information

Other information: This safety data sheet is prepared in accordance with Commission Regulation (EU) No 453/2010.

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* Data predicted using computational software. Toxtree - Toxic Hazard Estimation by decision tree approach. http://ecb.jrc.ec.europa.eu/qsar/qsar-tools/index.php?c=TOXTREE

~ Data predicted using computatioanl software ACD/ToxSuite v 2.95.1 Copyright 1994-2009 ACD/labs, Copyright 2001-2009 Pharma Algorithms, Inc, Advanced Chemistry Development, Inc (ACD/Labs). http://www.acdlabs.com/products/pc_admet/tox/tox/

Phrases used in s.2 and 3: H302+312+332: Harmful if swallowed, in contact with skin or if inhaled.
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H319: Causes serious eye irritation.
H335: May cause respiratory irritation.
R20/21/22: Harmful by inhalation, in contact with skin and if swallowed.
R36/37/38: Irritating to eyes, respiratory system and skin.

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