SAFETY DATA SHEET

1-(CHLOROMETHYL)-4-FLUORO-1,4-DIAZONIABICYCLO[2.2.2]OCTANE BIS(TETRAFLUOROBORATE)

Compilation date: 12/10/2008

Revision date: 18/05/2016

Revision No: 3

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

1.1. Product identifier

Product name: 1-(CHLOROMETHYL)-4-FLUORO-1,4-DIAZONIABICYCLO[2.2.2]OCTANE BIS (TETRAFLUOROBORATE)

CAS number: 140681-55-6

EINECS number: 414-380-4

Index number: 005-015-00-6

Product code: PC3728K

Synonyms: SELECTFLUOR

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 CLP: Self-heat. 2: H252; Aquatic Chronic 3: H412; Skin Sens. 1: H317; Acute Tox. 4: H302; Eye Dam. 1: H318

Most important adverse effects: Self-heating in large quantities; may catch fire. Causes serious eye damage. Harmful to aquatic life with long lasting effects. Harmful if swallowed. May cause an allergic skin reaction.

2.2. Label elements

Label elements:

Hazard statements: H252: Self-heating in large quantities; may catch fire.

[cont...]

H318: Causes serious eye damage.

H412: Harmful to aquatic life with long lasting effects.

H302: Harmful if swallowed.

H317: May cause an allergic skin reaction.

Signal words: Danger

Hazard pictograms: GHS02: Flame

GHS05: Corrosion

GHS07: Exclamation mark

Precautionary statements: P310: Immediately call a POISON CENTER/doctor/.

P260: Do not breathe dust.

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

2.3. Other hazards

Other hazards: This substance is categorised as self-heating.

PBT: This product is not identified as a PBT/vPvB substance.

Section 3: Composition/information on ingredients

3.1. Substances

Chemical identity: 1-(CHLOROMETHYL)-4-FLUORO-1,4-DIAZONIABICYCLO[2.2.2]OCTANE BIS (TETRAFLUOROBORATE)

CAS number: 140681-55-6

EINECS number: 414-380-4

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. Transfer to hospital for specialist examination.

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.

[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.

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

Immediate / special treatment: Hydrofluoric (HF) acid burns require immediate and specialized first aid and medical treatment. Symptoms may be delayed up to 24 hours depending on the concentration of HF. After decontamination with water,
further damage can occur due to penetration/ absorption of the fluoride ion. Treatment should be directed toward binding the fluoride ion as well as the effects of exposure. Skin exposures can be treated with a 2.5% calcium gluconate gel repeated until burning ceases. More serious skin exposures may require subcutaneous calcium gluconate except for digital areas unless the physician is experienced in this technique, due to the potential for tissue injury from increased pressure. Absorption can readily occur through the subungual areas and should be considered when undergoing decontamination. Prevention of
absorption of the fluoride ion in cases of ingestion can be obtained by giving milk, chewable calcium carbonate tablets or Milk of Magnesia to conscious victims. Conditions such as hypoc hypomagnesemia and cardiac arrhythmias should be monitored for, since they can occur after exposure.Consult a physician. Show this safety data sheet to the doctor in attendance.

Section 5: Fire-fighting measures

5.1. Extinguishing media

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

5.2. Special hazards arising from the substance or mixture

Exposure hazards: In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen oxides (NOx). Borane/boron oxides. Hydrogen chloride (HCl). Hydrogen fluoride (HF).

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.

[cont...]

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 a cool, well ventilated area. Keep container tightly closed. The floor of the storage room must be impermeable to prevent the escape of liquids. Moisture sensitive. Store under Argon. Recommended storage temp 2-8 ℃.

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.

DNEL/PNEC Values

DNEL / PNEC No data available.

8.2. Exposure controls

Engineering measures: Ensure there is sufficient ventilation of the area. The floor of the storage room must be impermeable to prevent the escape of liquids.

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

Hand protection: Protective gloves.

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

Skin protection: Protective clothing.

Section 9: Physical and chemical properties

[cont...]

9.1. Information on basic physical and chemical properties

State: Powder

Colour: White

Odour: Irritating odour

Oxidising: Oxidising (by EC criteria)

Solubility in water: Soluble

Melting point/range℃: 260

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. Moist air. Humidity.

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). Hydrogen chloride (HCl). Boron Oxides. Hydrogen fluoride (HF).

Section 11: Toxicological information

11.1. Information on toxicological effects

Toxicity values:

Route	Species	Test	Value	Units
ORAL	RAT	LD50	500	mg/kg
DERMAL	RAT	LD50	>2000	mg/kg

[cont...]

Relevant hazards for substance:

Hazard	Route	Basis
Acute toxicity (ac. tox. 4)	ING	Hazardous: calculated
Serious eye damage/irritation	OPT	Hazardous: calculated
Respiratory/skin sensitisation	DRM	Hazardous: calculated

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.

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.

Section 12: Ecological information

12.1. Toxicity

Ecotoxicity values:

Species	Test	Value	Units
Oncorhynchus mykiss (rainbow trout)	24H LC50	100	mg/l
Daphnia magna	48H EC50	25	mg/l

12.2. Persistence and degradability

Persistence and degradability: No data available.

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 product is not identified as a PBT/vPvB substance.

12.6. Other adverse effects

Other adverse effects: Harmful to aquatic organisms.

Section 13: Disposal considerations

13.1. Waste treatment methods

Disposal operations: Transfer to a suitable container and arrange for collection by specialised disposal company. 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.

[cont...]

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: * UN3088

14.2. UN proper shipping name

Shipping name: SELF-HEATING SOLID, ORGANIC, N.O.S.
(1-(Chloromethyl)-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane bis(tetrafluoroborate))

14.3. Transport hazard class(es)

Transport class: 4.2

14.4. Packing group

Packing group: * II

14.5. Environmental hazards

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

14.6. Special precautions for user

Tunnel code: D/E

Transport category: 2

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. The OECD QSAR-Toolbox for grouping chemicals into categories. Developed by LMC bulgaria.
http://echa.europa.eu/support/oecd-qsar-toolbox
~ Data predicted using computational 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 s.3: H252: Self-heating in large quantities; may catch fire.

[cont...]

H302: Harmful if swallowed.

H317: May cause an allergic skin reaction.

H318: Causes serious eye damage.

H412: Harmful to aquatic life with long lasting effects.

Legal disclaimer: The material is intended for research purposes only and should be handled exclusively by those who have been fully trained in safety, laboratory and chemical handling procedures. The above information is believed to be correct to the best of our knowledge. The above information is believed to be correct to the best of our knowledge at the date of its publication, but should not be considered to be all inclusive. It should be used only as a guide for safe handling, storage, transportation and disposal. We cannot guarantee that the hazards detailed in this document are the only hazards that exist for this product. This is not a warranty and Apollo Scientific Ltd shall not be held liable for any damage resulting from handling or from contact with the above product.