

Creation Date 13-Mar-2009

Revision Date 25-Aug-2023

Revision Number 5

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

1.1. Product identifier

Product Description: Cat No. : Molecular Formula 1-Propyl-1H-pyrazole-4-boronic acid, pinacol ester MAY00019DA; MAY00019ZZ C12 H21 B N2 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

Company

UK entity/business name

Thermo Fisher Scientific (Heysham), Shore Road, Port of Heysham Industrial Park, Heysham, Lancashire, LA3 2XY United Kingdom

EU entity/business name

Thermo Fisher Scientific Janssen Pharmaceuticalaan 3a 2440 Geel, Belgium

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 - Regulation (EC) No 1272/2008

 Physical hazards

 Flammable liquids
 Category 3 (H226)

 Health hazards

 Skin Corrosion/Irritation
 Category 2 (H315)

1-Propyl-1H-pyrazole-4-boronic acid, pinacol ester

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Category 2 (H319)

Category 3 (H335)

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

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

- H226 Flammable liquid and vapor
- H315 Causes skin irritation
- H319 Causes serious eye irritation
- H335 May cause respiratory irritation

Precautionary Statements

- P264 Wash face, hands and any exposed skin thoroughly after handling
- P337 + P313 If eye irritation persists: Get medical advice/attention
- P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing
- P312 Call a POISON CENTER or doctor if you feel unwell
- P280 Wear protective gloves/protective clothing/eye protection/face protection
- P332 + P313 If skin irritation occurs: Get medical advice/attention
- P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower
- P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

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 - Regulation (EC) No 1272/2008
1-Propyl-1H-pyrazole-4-boronic acid, pinacol ester	827614-69-7		>95	STOT SE 3 (H335) Skin Irrit. 2 (H315)
				Eye Irrit. 2 (H319) Flam. Liq. 3 (H226)

Full text of Hazard Statements: 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. 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.	
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		

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

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. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons No information available.

5.2. Special hazards arising from the substance or mixture

Flammable. Thermal decomposition can lead to release of irritating gases and vapors. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NOx), 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

1-Propyl-1H-pyrazole-4-boronic acid, pinacol ester

Use personal protective equipment as required. Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.

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

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

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. Avoid ingestion and inhalation. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take precautionary measures against static discharges.

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. Flammables area. Keep away from heat, sparks and flame.

Technical Rules for Hazardous Substances (TRGS) 510 Class 3 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)

1-Propyl-1H-pyrazole-4-boronic acid, pinacol ester

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No information available

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. Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment.

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

Natural rubber Ser Butyl rubber red Nitrile rubber Neoprene PVC	e manufacturers commendations	Glove thickness -	EU standard EN 374	Glove comments (minimum requirement)
Skin and body protection	n Long sle	eved 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 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 Recommended Filter type: Particulates filter conforming to EN 143 or Acid gases filter Type E Yellow conforming to EN14387
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:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141 When RPE is used a face piece Fit Test should be conducted

Environmental exposure controls

No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance Odor Odor Threshold Melting Point/Range Softening Point Boiling Point/Range Flammability (liquid) Flammability (solid,gas) Explosion Limits	Light yellow No information available No data available No data available No data available No information available Flammable Not applicable No information available	Estimated Liquid
Flash Point Autoignition Temperature Decomposition Temperature pH Viscosity Water Solubility Solubility in other solvents Partition Coefficient (n-octanol/wate Vapor Pressure Density / Specific Gravity	No information available °C / °F No data available No information available No information available No information available Immiscible No information available er) No information available No data available 0.996 @ 25°C / 77°F	Method - No information available
Bulk Density Vapor Density Particle characteristics	Not applicable No data available Not applicable (liquid)	Liquid (Air = 1.0)

9.2. Other information

Molecular Formula Molecular Weight Explosive Properties C12 H21 B N2 O2 236.12 explosive air/vapour mixtures possible

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity	None known, based on information available
10.2. Chemical stability	Stable under normal conditions.
10.3. Possibility of hazardous reaction	ons
Hazardous Polymerization Hazardous Reactions	Hazardous polymerization does not occur. None under normal processing.
10.4. Conditions to avoid	Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition.
10.5. Incompatible materials	Strong oxidizing agents.

10.6. Hazardous decomposition products

1-Propyl-1H-pyrazole-4-boronic acid, pinacol ester

Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NOx). Oxides of boron.

SECTION 11: TOXICOLOGICAL INFORMATION

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

Product Information	No acute toxicity information is available for this product	
(a) acute toxicity; Oral Dermal Inhalation	No data available 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; Results / Target organs	Category 3 Respiratory system.	
(i) STOT-repeated exposure;	No data available	
Target Organs	No information available.	
(j) aspiration hazard;	No data available	
Symptoms / effects both acute and	Symptoms of overexposure may be headache dizziness tiredness pausea an	

Symptoms / effects, both acute and Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting. delayed

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

1-Propyl-1H-pyrazole-4-boronic acid, pinacol ester

degradable in waste water treatment plants.

12.2. Persistence and degradability Persistence	Immiscible with water.
12.3. Bioaccumulative potential	May have some potential to bioaccumulate
<u>12.4. Mobility in soil</u>	Spillage unlikely to penetrate soil Is not likely mobile in the environment due its low water solubility.
12.5. Results of PBT and vPvB assessment	No data available for assessment.
<u>12.6. Endocrine disrupting</u> properties Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors

<u>12.7. Other adverse effects</u> 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

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. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.
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 flush to sewer. Can be landfilled or incinerated, when in compliance with local regulations.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

<u>14.1. UN number</u>	UN1993
14.2. UN proper shipping name	Flammable liquid, n.o.s.
Technical Shipping Name	1-Propyl-1H-pyrazole-4-boronic acid, pinacol ester
14.3. Transport hazard class(es)	3
14.4. Packing group	III

1-Propyl-1H-pyrazole-4-boronic acid, pinacol ester

ADR

<u>14.1. UN number</u> <u>14.2. UN proper shipping name</u> Technical Shipping Name <u>14.3. Transport hazard class(es)</u> <u>14.4. Packing group</u>	UN1993 Flammable liquid, n.o.s. 1-Propyl-1H-pyrazole-4-boronic acid, pinacol ester 3 III
IATA	
<u>14.1. UN number</u> <u>14.2. UN proper shipping name</u> Technical Shipping Name <u>14.3. Transport hazard class(es)</u> <u>14.4. Packing group</u>	UN1993 Flammable liquid, n.o.s. 1-Propyl-1H-pyrazole-4-boronic acid, pinacol ester 3 III
14.5. Environmental hazards	No hazards identified
14.6. Special precautions for user	No special precautions required.
<u>14.7. Maritime transport in bulk</u> 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 (TCSI), 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)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
1-Propyl-1H-pyrazole-4-boronic acid, pinacol ester	827614-69-7	-	-	-	-	-	-	-	-
Component	CAS No	TSCA	TSCA In notific Active-I	ation -	DSL	NDSL	AICS	NZIoC	PICCS
1-Propyl-1H-pyrazole-4-boronic	827614-69-7					_			

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 Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
1-Propyl-1H-pyrazole-4-boronic acid, pinacol ester	827614-69-7	-	-	-

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report		
		Notification	Requirements		
1-Propyl-1H-pyrazole-4-boro	827614-69-7	Not applicable	Not applicable		

1-Propyl-1H-pyrazole-4-boronic acid, pinacol ester

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nic acid, pinacol ester

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

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

H226 - Flammable liquid and vapor

Legend

CAS - Chemical Abstracts Service	TSCA - United States Toxic Substances Control Act Section 8(b) Inventory
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	TWA - Time Weighted Average
ACGIH - American Conference of Governmental Industrial Hygienists	IARC - International Agency for Research on Cancer
DNEL - Derived No Effect Level	Predicted No Effect Concentration (PNEC)
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

Ships

Transport Association

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

1-Propyl-1H-pyrazole-4-boronic acid, pinacol ester

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ICAO/IATA - International Civil Aviation Organization/International Air

MARPOL - International Convention for the Prevention of Pollution from

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

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.

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Revision Summary	SDS sections updated, 1, 2, 9, 11, 12, 15, 16.

This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006. COMMISSION REGULATION (EU) 2020/878 amending Annex II to Regulation (EC) No 1907/2006

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