

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

Cat No. : MAY00019DA; MAY00019ZZ

Molecular Formula 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

EU entity/business name Thermo Fisher Scientific Janssen Pharmaceuticalaan 3a

2440 Geel, Belgium

UK entity/business name

Thermo Fisher Scientific (Heysham),

Shore Road,

Port of Heysham Industrial Park, Heysham, Lancashire, LA3 2XY

United Kingdom

Swiss distributor - Fisher Scientific AG Neuhofstrasse 11. CH 4153 Reinach

Tel: +41 (0) 56 618 41 11

e-mail - infoch@thermofisher.com

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

customers in Switzerland:

Tox Info Suisse Emergency Number: 145 (24hr)

Tox Info Suisse: +41-44 251 51 51 (Emergency number from abroad)

Chemtrec (24h) Toll-Free: 0800 564 402 Chemtrec Local: +41-43 508 20 11 (Zurich)

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

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

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

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

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.

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

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

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 Storage Class (LGK) (Germany)

Class 3

Switzerland - Storage of hazardous substances

Storage class - SC 3

https://www.kvu.ch/de/themen/stoffe-und-produkte https://www.kvu.ch/fr/themes/substances-et-produits https://www.kvu.ch/it/temi/sostanze-e-prodotti

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

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

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.

MDHS70 General methods for sampling airborne gases and vapours

MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography

MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

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

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

Eve Protection Goggles (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Natural rubber	See manufacturers	-		(minimum requirement)

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Butyl rubber recommendations EN 374
Nitrile rubber
Neoprene
PVC

Skin and body protection Long sleeved clothing.

Inspect gloves before use. observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information) 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. 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

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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 Light yellow

Odor
No information available
Odor Threshold
No data available
Melting Point/Range
No data available
Softening Point
No data available
No information available
No information available

Flammability (liquid)FlammableEstimatedFlammability (solid,gas)Not applicableLiquid

Explosion Limits No information available

Flash Point No information available °C / °F Method - No information available

Autoignition Temperature No data available

Decomposition Temperature
pHNo information available
No information available
No information available
No information available
Immiscible

water Solubility Infinisciple

Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

Vapor Pressure No information available

Density / Specific Gravity No data available 0.996 @ 25°C /

77°F

Bulk DensityNot applicableLiquidVapor DensityNo data available(Air = 1.0)

Particle characteristics Not applicable (liquid)

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

9.2. Other information

Molecular Formula C12 H21 B N2 O2

Molecular Weight 236.12

Explosive Properties 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 reactions

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous Reactions 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

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 InformationNo acute toxicity information is available for this product

(a) acute toxicity;

OralNo data availableDermalNo data availableInhalationNo 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

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

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There are no known carcinogenic chemicals in this product

No data available (g) reproductive toxicity;

Category 3 (h) STOT-single exposure;

Results / Target organs Respiratory system.

No data available (i) STOT-repeated exposure;

No information available. **Target Organs**

No data available (j) aspiration hazard;

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

delayed

11.2. Information on other hazards

Assess endocrine disrupting properties for human health. This product does not contain any **Endocrine Disrupting Properties**

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

Persistence Immiscible with water.

12.3. Bioaccumulative potential May have some potential to bioaccumulate

Spillage unlikely to penetrate soil Is not likely mobile in the environment due its low water 12.4. Mobility in soil

solubility.

12.5. Results of PBT and vPvB

assessment

No data available for assessment.

12.6. Endocrine disrupting

properties

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

12.7. Other adverse effects

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

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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.

Dispose of this container to hazardous or special waste collection point. Empty containers **Contaminated Packaging**

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.

Disposal should be in accordance with applicable regional, national and local laws and **Switzerland - Waste Ordinance**

regulations. Ordinance on the Avoidance and the Disposal of Waste (Waste Ordinance,

ADWO) SR 814.600

https://www.fedlex.admin.ch/eli/cc/2015/891/en

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number 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)

14.4. Packing group Ш

ADR

UN1993 14.1. UN number

14.2. UN proper shipping name Flammable liquid, n.o.s.

1-Propyl-1H-pyrazole-4-boronic acid, pinacol ester **Technical Shipping Name**

3 14.3. Transport hazard class(es) 14.4. Packing group Ш

IATA

14.1. UN number 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 Ш

No hazards identified 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 (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	827614-69-7	-	-	-	-	-	-	-	-
acid pinacol ester									

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
1-Propyl-1H-pyrazole-4-boronic acid pinacol ester	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	J	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 Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements
1-Propyl-1H-pyrazole-4-boro nic acid pinacol ester	827614-69-7	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)

Swiss Regulations

Article 4 para. 4 of the Ordinance on the protection of young people in the workplace (SR 822.115) and Article 1 lit. f of the EAER regulation on hazardous work and young people (SR 822.115.2).

Take note on Article 13 Maternity Ordinance (SR 822.111.52) with regards expectant and nursing mothers.

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 DSL/NDSL - Canadian Domestic Substances List/Non-Domestic

Substances/EU List of Notified Chemical Substances

Substances List

PICCS - Philippines Inventory of Chemicals and Chemical Substances IECSC - Chinese Inventory of Existing Chemical Substances **KECL** - Korean Existing and Evaluated Chemical Substances

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.

Creation Date 13-Mar-2009 **Revision Date** 25-Aug-2023

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

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

For Switzerland - Compiled in accordance with the technical provisions referred to in Annex 2, Number 3, ChemO (SR 813.11 - Ordinance on Protection against Dangerous Substances and Preparations).

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