

Creation Date 06-Jun-2011 Revision Date 14-Feb-2013 Revision Number 3

# SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

**Product Identifier** 

Product Description: 1-Isobutyl-1H-pyrazole-4-boronic acid pinacol ester

Cat No. 439730000; 439730010; 439730050

Synonyms 1-lsobutyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-pyrazole

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

Recommended Use Laboratory chemicals
Uses advised against No Information available

Details of the supplier of the safety data sheet

Company

Acros Organics BVBA Janssen Pharmaceuticalaan 3a

2440 Geel, Belgium

E-mail address begel.sdsdesk@thermofisher.com

**Emergency Telephone Number** 

For information in the US, call: 001-800-ACROS-01 For information in Europe, call: +32 14 57 52 11

Emergency Number, Europe: +32 14 57 52 99 Emergency Number, US: 001-201-796-7100

CHEMTREC Phone Number, US: 001-800-424-9300 CHEMTREC Phone Number, Europe: 001-703-527-3887

# **SECTION 2. HAZARDS IDENTIFICATION**

# Classification of the substance or mixture REGULATION (EC) No 1272/2008

` '	
Skin Corrosion/irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity - (single exposure)	Category 3
Flammable liquids	Category 3

# Classification according to EU Directives 67/548/EEC or 1999/45/EC

For the full text of the R-phrases and H-Statements mentioned in this Section, see Section 16

Symbol(s) Xi - Irritant R-phrase(s) R10 - Flammable

Risk Combination Phrases R36/37/38 - Irritating to eyes, respiratory system and skin

# **Label Elements**



1-Isobutyl-1H-pyrazole-4-boronic acid pinacol ester

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# **SECTION 2. HAZARDS IDENTIFICATION**



Signal Word

Warning

# **Hazard Statements**

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

H226 - Flammable liquid and vapor

## Precautionary Statements - EU (§28, 1272/2008)

P210 - Keep away from heat/sparks/open flames/hot surfaces. - No smoking

P261 - Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray

P280 - Wear protective gloves/ protective clothing/ eye protection/ face protection

P303 + P361 + P353 - IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower

P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

## Other Hazards

No information available.

# **SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Component	EC-No.	Weight %	CAS-No	67/548/EEC Classification	CLP Classification - Regulation (EC) No 1272/2008	REACH No.
1-Isobutyl-1H-pyrazole-4-boronic acid pinacol ester 827614-66-4		>95	827614-66-4	Xi; R36/37/38 R10	Flam. Liq. 3 (H226) Eye Irrit. 2 (H319) STOT SE 3 (H335) Skin Irrit. 2 (H315)	-

For the full text of the R-phrases and H-Statements mentioned in this Section, see Section 16



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#### **SECTION 4. FIRST AID MEASURES**

Description of first aid measures

Eye Contact Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get

medical attention immediately if symptoms occur.

**Skin Contact** Wash off immediately with plenty of water for at least 15 minutes. Remove and wash

contaminated clothing before re-use. Get medical attention if symptoms occur..

**Ingestion** Do not induce vomiting. Clean mouth with water and drink afterwards plenty of water. Get

medical attention if symptoms occur..

**Inhalation** Move to fresh air. Get medical attention immediately if symptoms occur. If breathing is difficult,

give oxygen.

**Protection of First-aiders** 

Notes to Physician

Use personal protective equipment. Remove all sources of ignition

Treat symptomatically

## **SECTION 5. FIRE-FIGHTING MEASURES**

#### **Extinguishing media**

#### Suitable Extinguishing Media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide. Cool closed containers exposed to fire with water spray.

#### Extinguishing media which must not be used for safety reasons

No information available.

#### Special hazards arising from the substance or mixture

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

#### Advice for fire-fighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

# **SECTION 6. ACCIDENTAL RELEASE MEASURES**

#### Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Remove all sources of ignition. Take precautionary measures against static discharges.

## **Environmental precautions**

Should not be released into the environment.

#### 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.



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## SECTION 7. HANDLING AND STORAGE

#### **Precautions for Safe Handling**

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

# 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 and sources of ignition.

#### **Specific End Uses**

# SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Control parameters

This product, as supplied, does not contain any hazardous materials with occupational **Exposure limits** 

exposure limits established by the region specific regulatory bodies.

This product, as supplied, does not contain any hazardous materials with biological limits **Biological limit values** 

established by the region specific regulatory bodies.

**Derived No Effect Level (DNEL)** 

**Predicted No Effect Concentration** 

(PNEC)

No information available. No information available.

**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

Personal protective equipment

**Eve Protection Hand Protection** 

Skin and body protection

**Respiratory Protection** 

Goaales

Protective gloves Wear appropriate protective gloves and clothing to prevent skin exposure

Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN

149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits

are exceeded or if irritation or other symptoms are experienced

**Hygiene Measures** 

Handle in accordance with good industrial hygiene and safety practice

No information available. **Environmental exposure controls** 

# **SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES**

**Physical State** Liquid **Appearance** Pale yellow

Odor No information available рH No information available.

248 - 249°C / 478.4 - 480.2°F @ 760 mmHg **Boiling Point/Range** Melting Point/Range No data available

Flash Point 48°C / 118.4°F

**Autoignition Temperature** No information available.



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## **SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES**

Water SolubilityInsoluble in waterDensity1.003 @ 25°CMolecular FormulaC13 H23 B N2 O2

Molecular Weight 250.15

# **SECTION 10. STABILITY AND REACTIVITY**

#### Reactivity

## **Chemical Stability**

Stable under normal conditions.

# **Possibility of Hazardous Reactions**

**Hazardous Polymerization Hazardous Reactions .**Hazardous polymerization does not occur.

None under normal processing..

**Conditions to Avoid** 

Incompatible products, Excess heat, Keep away from open flames, hot surfaces and sources of ignition.

#### **Incompatible Materials**

Strong oxidizing agents, Strong acids, Strong bases.

#### **Hazardous Decomposition Products**

Thermal decomposition can lead to release of irritating gases and vapors. Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Nitrogen oxides (NOx). Oxides of boron.

## **SECTION 11. TOXICOLOGICAL INFORMATION**

#### Information on Toxicological Effects

**Acute Toxicity** 

Product Information No acute toxicity information is available for this product

**Component Information** 

**Chronic Toxicity** 

Carcinogenicity There are no known carcinogenic chemicals in this product

SensitizationNo information available.Mutagenic EffectsNo information availableReproductive EffectsNo information available.Developmental EffectsNo information available.Target OrgansSkin Respiratory system Eyes

**Endocrine Disruptor Information** None known



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**SECTION 12. ECOLOGICAL INFORMATION** 

**Toxicity** 

**Ecotoxicity effects**Contains no substances known to be hazardous to the environment or that are not degradable

in waste water treatment plants

Persistence and degradability

No information available

**Bioaccumulative potential** 

No information available.

**Mobility in soil** 

No information available.

Results of PBT and vPvB assessment

Other adverse effects

No information available

# **SECTION 13. DISPOSAL CONSIDERATIONS**

Waste treatment methods

Waste from Residues / Unused

**Products** 

Dispose of in accordance with local regulations

Contaminated Packaging Empty containers should be taken to local recyclers for disposal

# **SECTION 14. TRANSPORT INFORMATION**

#### IMDG/IMO

UN-No 1993 Hazard Class 3 Packing Group III

**Proper Shipping Name** Flammable liquid, n.o.s.

**ADR** 

UN-No 1993 Hazard Class 3 Packing Group III

Proper Shipping Name FLAMMABLE LIQUID, N.O.S.

**IATA** 

UN-No 1993 Hazard Class 3 Packing Group III

Proper Shipping Name FLAMMABLE LIQUID, N.O.S.\*



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## **SECTION 15. REGULATORY INFORMATION**

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

#### **International Inventories**

#### Legend

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

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

PICCS - Philippines Inventory of Chemicals and Chemical Substances

**ENCS** - Japan Existing and New Chemical Substances

**IECSC** - China Inventory of Existing Chemical Substances

**AICS** - Inventory of Chemical Substances

**KECL** - Existing and Evaluated Chemical Substances

## **Chemical Safety Assessment**

# **SECTION 16. OTHER INFORMATION**

#### Full text of R-phrases referred to under sections 2 and 3

R10 - Flammable

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

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

H226 - Flammable liquid and vapor

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

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**Revision Summary** 

**Reason for revision** (M)SDS sections updated, 2, 3, 4, 8, 16.

This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006

Disclaimer

The information provided on 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 guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as 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 material or in any process, unless specified in the text.

**End of Safety Data Sheet**