

## Chemical Safety Data Sheet MSDS / SDS

**1-ISOBUTYL-4-(4,4,5,5-TETRAMETHYL-1,3,2-DIOXABOROLAN-2-YL)-1H-PYRAZOLE**

Revision Date:2023-11-29 Revision Number:1

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name : 1-ISOBUTYL-4-(4,4,5,5-TETRAMETHYL-1,3,2-DIOXABOROLAN-2-YL)-1H-PYRAZOLE  
CBnumber : CB2272395  
CAS : 827614-66-4  
Synonyms : 1-isobutyl-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**

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 400-158-6606

**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

**Precautionary statements**

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

**Hazard statements**

H226 Flammable liquid and vapour  
H315 Causes skin irritation  
H319 Causes serious eye irritation

**SECTION 3: Composition/information on ingredients****Substance**

Product name	: 1-ISOBUTYL-4-(4,4,5,5-TETRAMETHYL-1,3,2-DIOXABOROLAN-2-YL)-1H-PYRAZOLE
Synonyms	: 1-isobutyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-pyrazole
CAS	: 827614-66-4
MF	: C13H23BN2O2
MW	: 250.14

---

## SECTION 4: First aid measures

### **Most important symptoms and effects, both acute and delayed**

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

### **Indication of any immediate medical attention and special treatment needed**

No data available

---

## SECTION 5: Firefighting measures

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

Carbon oxides, Nitrogen oxides (NOx), Borane/boron oxides

### **Advice for firefighters**

No data available

### **Further information**

No data available

---

## SECTION 6: Accidental release measures

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

For personal protection see section 8.

### **Environmental precautions**

No data available

### **Methods and materials for containment and cleaning up**

No data available

### **Reference to other sections**

For disposal see section 13.

---

## SECTION 7: Handling and storage

## Precautions for safe handling

For precautions see section 2.2.

## Conditions for safe storage, including any incompatibilities

No data available

## Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

---

## SECTION 8: Exposure controls/personal protection

### control parameter

#### Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

---

## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	liquid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	No data available
Initial boiling point and boiling range	248 - 249 °C - lit.
Flash point	47 °C
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available
Relative density	1,003 g/cm <sup>3</sup> at 25 °C
Water solubility	No data available
Partition coefficient: n-octanol/water	log Pow: 3,355
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

### Other safety information

No data available

---

## SECTION 10: Stability and reactivity

### **Reactivity**

No data available

### **Chemical stability**

No data available

### **Possibility of hazardous reactions**

No data available

### **Conditions to avoid**

No data available

### **Incompatible materials**

Strong oxidizing agents, Halogens, Mineral acids

### **Hazardous decomposition products**

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx), Borane/boron oxides

Other decomposition products - No data available

In the event of fire: see section 5

---

## SECTION 11: Toxicological information

### **Information on toxicological effects**

#### **Acute toxicity**

No data available

#### **Skin corrosion/irritation**

No data available

#### **Serious eye damage/eye irritation**

No data available

#### **Respiratory or skin sensitisation**

No data available

#### **Germ cell mutagenicity**

No data available

#### **Carcinogenicity**

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

#### **Reproductive toxicity**

No data available

#### **Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

---

## SECTION 12: Ecological information

**Toxicity**

No data available

**Persistence and degradability**

No data available

**Bioaccumulative potential**

No data available

**Mobility in soil**

No data available

**Results of PBT and vPvB assessment**

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

**Other adverse effects**

No data available

---

## SECTION 13: Disposal considerations

**Waste treatment methods**

**Product**

No data available

---

## SECTION 14: Transport information

**UN number**

ADR/RID: 1993 IMDG: 1993 IATA: 1993

## UN proper shipping name

ADR/RID: FLAMMABLE LIQUID, N.O.S. (1-Isobutylpyrazole-4-boronic acid pinacol ester) IMDG: FLAMMABLE LIQUID, N.O.S. (1-Isobutylpyrazole-4-boronic acid pinacol ester) IATA: Flammable liquid, n.o.s. (1-Isobutylpyrazole-4-boronic acid pinacol ester)

## Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA: 3

## Packaging group

ADR/RID: III IMDG: III IATA: III

## Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

## Special precautions for user

No data available

---

## SECTION 15: Regulatory information

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

#### Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

#### Measures for Environmental Management of New Chemical Substances

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: <https://www.mee.gov.cn/>

EC Inventory:Not Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Not Listed. website: <https://echa.europa.eu/>

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: <https://www.epa.govt.nz/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: <https://emb.gov.ph/>

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: <https://www.epa.gov/>

Vietnam National Chemical Inventory:Not Listed. website: <https://chemicaldata.gov.vn/>

---

## SECTION 16: Other information

### Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

## References

- 【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- 【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- 【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>
- 【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:  
[http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)
- 【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- 【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

### Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.