

**SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING****1.1. Product identifier**

**Product Description:** 1-Isobutyl-1H-pyrazole-4-boronic acid pinacol ester  
**Cat No. :** 439730000; 439730010; 439730050  
**Synonyms**  
**Molecular Formula** 1-Isobutyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-pyrazole  
C13 H23 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**  
Fisher Scientific UK  
Bishop Meadow Road,  
Loughborough, Leicestershire LE11 5RG, United Kingdom

**Swiss distributor** - Fisher Scientific AG  
Neuhofstrasse 11, CH 4153 Reinach  
Tel: +41 (0) 56 618 41 11  
e-mail - [infoch@thermofisher.com](mailto:infoch@thermofisher.com)

**E-mail address** [begel.sdsdesk@thermofisher.com](mailto: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**

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## CLP Classification - Regulation (EC) No 1272/2008

### Physical hazards

Flammable liquids Category 3 (H226)

### Health hazards

Skin Corrosion/Irritation Category 2 (H315)  
Serious Eye Damage/Eye Irritation Category 2 (H319)  
Specific target organ toxicity - (single exposure) 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**

### 3.1. Substances

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

*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** Use personal protective equipment as required. Remove all sources of ignition.

### 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. Symptoms may be delayed.

## SECTION 5: FIREFIGHTING MEASURES

### 5.1. Extinguishing media

#### **Suitable Extinguishing Media**

Water spray, carbon dioxide (CO<sub>2</sub>), 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. 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**

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Thermal decomposition can lead to release of irritating gases and vapors, Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Nitrogen oxides (NO<sub>x</sub>), 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. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Ensure adequate ventilation. 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**

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## 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**

#### **Eye Protection**

Goggles (European standard - EN 166)

#### **Hand Protection**

Protective gloves

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

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Viton (R)	recommendations	EN 374
<b>Skin and body protection</b>	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 compatibility, 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.

<b>Respiratory Protection</b>	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
<b>Large scale/emergency use</b>	Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced <b>Recommended Filter type:</b> Organic gases and vapours filter Type A Brown conforming to EN14387
<b>Small scale/Laboratory use</b>	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. <b>Recommended half mask:-</b> Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141 When RPE is used a face piece Fit Test should be conducted
<b>Environmental exposure controls</b>	No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

### 9.1. Information on basic physical and chemical properties

<b>Physical State</b>	Liquid	
<b>Appearance</b>	Pale yellow	
<b>Odor</b>	No information available	
<b>Odor Threshold</b>	No data available	
<b>Melting Point/Range</b>	No data available	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	248 - 249 °C / 478.4 - 480.2 °F	@ 760 mmHg
<b>Flammability (liquid)</b>	Flammable	On basis of test data
<b>Flammability (solid,gas)</b>	Not applicable	Liquid
<b>Explosion Limits</b>	No data available	
<b>Flash Point</b>	48 °C / 118.4 °F	<b>Method -</b> No information available
<b>Autoignition Temperature</b>	No data available	
<b>Decomposition Temperature</b>	No data available	
<b>pH</b>	No information available	
<b>Viscosity</b>	No data available	
<b>Water Solubility</b>	Insoluble in water	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Vapor Pressure</b>	No data available	
<b>Density / Specific Gravity</b>	No data available	1.003 @ 25°C
<b>Bulk Density</b>	Not applicable	Liquid
<b>Vapor Density</b>	No data available	(Air = 1.0)
<b>Particle characteristics</b>	Not applicable (liquid)	

### 9.2. Other information

<b>Molecular Formula</b>	C13 H23 B N2 O2
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**Molecular Weight** 250.15  
**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. Strong acids. Strong bases.

**10.6. 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 (NO<sub>x</sub>). 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 No data available  
Dermal No data available  
Inhalation No 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

There are no known carcinogenic chemicals in this product

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(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3

Results / Target organs 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 delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting.

## 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 degradable in waste water treatment plants.

### 12.2. Persistence and degradability

**Persistence** Insoluble in water, May persist, based on information available.

### 12.3. Bioaccumulative potential

May have some potential to bioaccumulate

### 12.4. Mobility in soil

Spillage unlikely to penetrate soil The product evaporates slowly Is not likely mobile in the environment due its low water solubility. Spillage unlikely to penetrate soil

### 12.5. Results of PBT and vPvB assessment

No data available for assessment.

### 12.6. Endocrine disrupting properties

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

### 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

## **SECTION 13: DISPOSAL CONSIDERATIONS**

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## 13.1. Waste treatment methods

<b>Waste from Residues/Unused Products</b>	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.
<b>Contaminated Packaging</b>	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.
<b>European Waste Catalogue (EWC)</b>	According to the European Waste Catalog, Waste Codes are not product specific, but application specific.
<b>Other Information</b>	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.
<b>Switzerland - Waste Ordinance</b>	Disposal should be in accordance with applicable regional, national and local laws and regulations. Ordinance on the Avoidance and the Disposal of Waste (Waste Ordinance, ADWO) SR 814.600 <a href="https://www.fedlex.admin.ch/eli/cc/2015/891/en">https://www.fedlex.admin.ch/eli/cc/2015/891/en</a>

## **SECTION 14: TRANSPORT INFORMATION**

### IMDG/IMO

<b>14.1. UN number</b>	UN1993
<b>14.2. UN proper shipping name</b>	Flammable liquid, n.o.s.
<b>14.3. Transport hazard class(es)</b>	3
<b>14.4. Packing group</b>	III

### ADR

<b>14.1. UN number</b>	UN1993
<b>14.2. UN proper shipping name</b>	Flammable liquid, n.o.s.
<b>14.3. Transport hazard class(es)</b>	3
<b>14.4. Packing group</b>	III

### IATA

<b>14.1. UN number</b>	UN1993
<b>14.2. UN proper shipping name</b>	FLAMMABLE LIQUID, N.O.S.*
<b>14.3. Transport hazard class(es)</b>	3
<b>14.4. Packing group</b>	III

<b>14.5. Environmental hazards</b>	No hazards identified
<b>14.6. Special precautions for user</b>	No special precautions required.
<b>14.7. Maritime transport in bulk according to IMO instruments</b>	Not applicable, packaged goods

## **SECTION 15: REGULATORY INFORMATION**

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

### International Inventories

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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-Isobutyl-1H-pyrazole-4-boronic acid pinacol ester	827614-66-4	-	-	-	-	-	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
1-Isobutyl-1H-pyrazole-4-boronic acid pinacol ester	827614-66-4	-	-	-	-	-	-	-

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 (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
1-Isobutyl-1H-pyrazole-4-boronic acid pinacol ester	827614-66-4	-	-	-

## Seveso III Directive (2012/18/EC)

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-Isobutyl-1H-pyrazole-4-boronic acid pinacol ester	827614-66-4	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

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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

**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

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory  
**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List  
**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.

Fire prevention and fighting, identifying hazards and risks, static electricity, explosive atmospheres posed by vapours and dusts.  
Chemical incident response training.

**Creation Date** 06-Jun-2011  
**Revision Date** 13-Oct-2023  
**Revision Summary** Not applicable.

**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).**

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## 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**