

Revision Date 25-Aug-2023 Revision Number 4

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

1.1. Product identifier

Product Description: <u>1-(4-Bromobenzyl)-5-methyl-1H-1,2,3-triazole-4-carboxylic acid</u>

Cat No.: MO07389CB; MO07389DA; MO07389DE; MO07389FL; MO07389ZZ

Molecular Formula C11 H10 Br N3 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 .

y 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 solids Category 2 (H228)

**Health hazards** 

Skin Corrosion/Irritation Category 2 (H315)

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## 1-(4-Bromobenzyl)-5-methyl-1H-1,2,3-triazole-4-carboxylic acid

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Serious Eye Damage/Eye Irritation

Specific target organ toxicity - (single exposure)

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**

H228 - Flammable solid

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

## **Precautionary Statements**

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water

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

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-(4-Bromobenzyl)-5-methyl-1H-1,2,3-triazo le-4-carboxylic acid	845885-94-1		97	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Flam. Sol. 2 (H228)

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. Get medical attention if

symptoms occur.

**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

None reasonably foreseeable.

#### 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 (CO<sub>2</sub>). Dry chemical. Chemical foam.

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

No information available.

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

Flammable. Combustible material.

#### **Hazardous Combustion Products**

Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO2), Hydrogen halides, Bromine.

## 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

Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.

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## 1-(4-Bromobenzyl)-5-methyl-1H-1,2,3-triazole-4-carboxylic acid

#### 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

Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

#### 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. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Avoid dust formation.

#### **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 in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Flammables area.

Technical Rules for Hazardous Substances (TRGS) 510 Class 4.1B 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)

No information available

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#### **Predicted No Effect Concentration (PNEC)**

No information available.

## 8.2. Exposure controls

## **Engineering Measures**

Use explosion-proof electrical/ventilating/lighting equipment. Ensure that eyewash stations and safety showers are close to the workstation location.

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)

Protective gloves **Hand Protection** 

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Natural rubber	See manufacturers	-	EN 374	(minimum requirement)
Butyl rubber	recommendations			
Nitrile rubber				
Neoprene				
PVC				

Skin and body protection Long sleeved 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

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits Large scale/emergency use

are exceeded or if irritation or other symptoms are experienced Recommended Filter type: Particulates filter conforming to EN 143

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure Small scale/Laboratory use

limits are exceeded or if irritation or other symptoms are experienced.

Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN

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

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1-(4-Bromobenzyl)-5-methyl-1H-1,2,3-triazole-4-carboxylic acid

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Physical State Solid

Appearance White

Odor No information available
Odor Threshold No data available

Melting Point/Range 192 - 193 °C / 377.6 - 379.4 °F

Softening Point No data available
Boiling Point/Range No information available

Flammability (liquid) Not applicable Solid

Flammability (solid,gas)

Explosion Limits

No information available

No data available

Flash Point No information available Method - No information available

Autoignition TemperatureNo data availableDecomposition TemperatureNo data availablepHNo data available

Viscosity Not applicable Solid

Water Solubility Soluble in water

Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

Vapor PressureNo data availableDensity / Specific GravityNo data availableBulk DensityNo data available

Vapor Density Not applicable Solid

Particle characteristics No data available

9.2. Other information

Molecular Formula C11 H10 Br N3 O2

Molecular Weight 296.12

Flammable solids Burning rate or burning time = > 2.2 mm/s or < 45 secs

Wetted zone passed - No

Evaporation Rate Not applicable - Solid

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 PolymerizationNo information available.Hazardous ReactionsNone under normal processing.

10.4. Conditions to avoid

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

10.5. Incompatible materials

Strong oxidizing agents. Strong bases. Amines. Strong reducing agents.

10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Hydrogen halides.

Bromine.

**SECTION 11: TOXICOLOGICAL INFORMATION** 

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## 1-(4-Bromobenzyl)-5-methyl-1H-1,2,3-triazole-4-carboxylic acid

## 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

(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; Not applicable

Solid

Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects,both acute and No information available.

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** Do not empty into drains.

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1-(4-Bromobenzyl)-5-methyl-1H-1,2,3-triazole-4-carboxylic acid

12.2. Persistence and degradability

Soluble in water, Persistence is unlikely, based on information available. Persistence

12.3. Bioaccumulative potential Bioaccumulation is unlikely

The product is water soluble, and may spread in water systems. Will likely be mobile in the 12.4. Mobility in soil

environment due to its water solubility. Highly mobile in soils

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 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

14.1. UN number UN1325

14.2. UN proper shipping name Flammable solid, organic, n.o.s.

**Technical Shipping Name** 1-(4-Bromobenzyl)-5-methyl-1H-1,2,3-triazole-4-carboxylic acid

14.3. Transport hazard class(es) 4.1 14.4. Packing group

III

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1-(4-Bromobenzyl)-5-methyl-1H-1,2,3-triazole-4-carboxylic acid

ADR

**14.1. UN number** UN1325

**14.2. UN proper shipping name** Flammable solid, organic, n.o.s.

**Technical Shipping Name** 1-(4-Bromobenzyl)-5-methyl-1H-1,2,3-triazole-4-carboxylic acid

14.3. Transport hazard class(es) 4.1 14.4. Packing group III

**IATA** 

**14.1. UN number** UN1325

**14.2. UN proper shipping name** Flammable solid, organic, n.o.s.

**Technical Shipping Name** 1-(4-Bromobenzyl)-5-methyl-1H-1,2,3-triazole-4-carboxylic acid 4.1

14.4. Packing group

14.5. Environmental hazards No hazards identified

**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-(4-Bromobenzyl)-5-methyl-1H-1,	845885-94-1	-	-	-	-	-	-	-	-
2.3-triazole-4-carboxylic acid									

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
1-(4-Bromobenzyl)-5-methyl-1H-1, 2,3-triazole-4-carboxylic acid	845885-94-1	-	-	-	-	-	-	-

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-(4-Bromobenzyl)-5-methyl-1H-1,2, 3-triazole-4-carboxylic acid	845885-94-1	-	-	-

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-(4-Bromobenzyl)-5-methyl- 1H-1,2,3-triazole-4-carboxyli c acid		Not applicable	Not applicable

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1-(4-Bromobenzyl)-5-methyl-1H-1,2,3-triazole-4-carboxylic acid

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

H228 - Flammable solid

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

#### Legend

**CAS** - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical DSL/NDSL - Canadian Domestic Substances List/Non-Domestic 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

**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

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

IMO/IMDG - International Maritime Organization/International Maritime

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

Substances List

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

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

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

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

#### 1-(4-Bromobenzyl)-5-methyl-1H-1,2,3-triazole-4-carboxylic acid

Dangerous Goods Code MARPOL - International Convention for the Prevention of Pollution from

Ships

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

ATE - Acute Toxicity Estimate
VOC - (Volatile Organic Compound)

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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.

Revision Date 25-Aug-2023

**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**

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