

Creation Date 26-Feb-2010

Revision Date 25-Aug-2023

Revision Number 3

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

### 1.1. Product identifier

**Product Description:** tert-Butyl 4-[(trifluoromethyl)sulfonyloxy]-5,6-dihydropyridine-1(2H)-carboxylate  
**Cat No. :** MO07986DA; MO07986DE; MO07986ZZ  
**Molecular Formula** C11 H16 F3 N O5 S

### 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

**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 Pharmaceuticaaan 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

Based on available data, the classification criteria are not met

#### Health hazards

Acute oral toxicity

Category 4 (H302)

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Acute dermal toxicity  
Acute Inhalation Toxicity - Dusts and Mists  
Skin Corrosion/Irritation  
Serious Eye Damage/Eye Irritation  
Specific target organ toxicity - (single exposure)

Category 4 (H312)  
Category 4 (H332)  
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**

H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation  
H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled

## **Precautionary Statements**

P280 - Wear protective gloves/protective clothing/eye protection/face protection  
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water  
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray  
P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell  
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing  
P280 - Wear protective gloves/protective clothing/eye protection/face protection  
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

## **2.3. Other hazards**

This product does not contain any known or suspected endocrine disruptors

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

Component	CAS No	EC No	Weight %	CLP Classification - Regulation (EC) No 1272/2008
tert-Butyl 4-[(trifluoromethyl)sulfonyloxy]-5,6-dihydropyridine-1(2H)-carboxylate	138647-49-1		90	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Acute Tox. 4 (H302) Acute Tox. 4 (H312) Acute Tox. 4 (H332)

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Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
<b>Ingestion</b>	Do NOT induce vomiting. Call a physician or poison control center immediately.
<b>Inhalation</b>	Remove to fresh air. If breathing is difficult, give oxygen. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.
<b>Self-Protection of the First Aider</b>	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

No information available.

### 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, alcohol-resistant foam.

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

No information available.

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

Thermal decomposition can lead to release of irritating gases and vapors.

#### Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Nitrogen oxides (NO<sub>x</sub>), Hydrogen halides, Sulfur oxides.

### 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. Thermal decomposition can lead to release of irritating gases and vapors.

## SECTION 6: ACCIDENTAL RELEASE MEASURES

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

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Ensure adequate ventilation. Use personal protective equipment as required.

## **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.

## **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**

Use only under a chemical fume hood. Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation.

#### **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.

**Technical Rules for Hazardous Substances (TRGS) 510**      Class 12  
**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 only under a chemical fume hood. 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

Wear safety glasses with side shields (or goggles) (European standard - EN 166)

#### Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Disposable gloves	See manufacturers recommendations	-	EN 374	(minimum requirement)

#### Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

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

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. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

#### Large scale/emergency use

In case of insufficient ventilation, wear suitable respiratory equipment

#### 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. 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

#### Odor

No information available

#### Odor Threshold

No data available

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Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	No information available	
Flammability (liquid)	No data available	
Flammability (solid,gas)	No information available	
Explosion Limits	No data available	
Flash Point	Not applicable	Method - No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	No data available	
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Vapor Pressure	No data available	
Density / Specific Gravity	No data available	
Bulk Density	No data available	
Vapor Density	No data available	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

## 9.2. Other information

Molecular Formula	C11 H16 F3 N O5 S
Molecular Weight	331.31

## 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.

### 10.5. Incompatible materials

Strong oxidizing agents. Strong acids. Strong bases.

### 10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Nitrogen oxides (NO<sub>x</sub>). Hydrogen halides. Sulfur oxides.

## 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
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(a) acute toxicity;

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Oral	No data available
Dermal	No data available
Inhalation	No data available

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

(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; No data available

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 No information available.

## 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 No information available

12.3. Bioaccumulative potential No information available

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<b>12.4. Mobility in soil</b>	No information available
<b>12.5. Results of PBT and vPvB assessment</b>	No data available for assessment.
<b>12.6. Endocrine disrupting properties</b> <b>Endocrine Disruptor Information</b>	This product does not contain any known or suspected endocrine disruptors
<b>12.7. Other adverse effects</b> <b>Persistent Organic Pollutant</b> <b>Ozone Depletion Potential</b>	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

<b>Waste from Residues/Unused Products</b>	Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.
<b>Contaminated Packaging</b>	Empty remaining contents. Dispose of in accordance with local regulations. Do not re-use empty containers.
<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.

## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

<b>14.1. UN number</b>	UN2810
<b>14.2. UN proper shipping name</b> <b>Technical Shipping Name</b>	Toxic liquid, organic, n.o.s. tert-Butyl 4-[(trifluoromethyl)sulfonyloxy]-5,6-dihydropyridine-1(2H)-carboxylate
<b>14.3. Transport hazard class(es)</b> <b>Subsidiary Hazard Class</b>	6.1 +
<b>14.4. Packing group</b>	III

### ADR

<b>14.1. UN number</b>	UN2810
<b>14.2. UN proper shipping name</b> <b>Technical Shipping Name</b>	Toxic liquid, organic, n.o.s. tert-Butyl 4-[(trifluoromethyl)sulfonyloxy]-5,6-dihydropyridine-1(2H)-carboxylate
<b>14.3. Transport hazard class(es)</b>	6.1
<b>14.4. Packing group</b>	III

### IATA



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<b>14.1. UN number</b>	UN2810
<b>14.2. UN proper shipping name</b>	Toxic liquid, organic, n.o.s.
<b>Technical Shipping Name</b>	tert-Butyl 4-[(trifluoromethyl)sulfonyloxy]-5,6-dihydropyridine-1(2H)-carboxylate
<b>14.3. Transport hazard class(es)</b>	6.1
<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

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
tert-Butyl 4-[(trifluoromethyl)sulfonyloxy]-5,6-dihydropyridine-1(2H)-carboxylate	138647-49-1	-	-	-	-	-	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
tert-Butyl 4-[(trifluoromethyl)sulfonyloxy]-5,6-dihydropyridine-1(2H)-carboxylate	138647-49-1	-	-	-	-	-	-	-

**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 (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)
tert-Butyl 4-[(trifluoromethyl)sulfonyloxy]-5,6-dihydropyridine-1(2H)-carboxylate	138647-49-1	-	-	-

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
tert-Butyl 4-[(trifluoromethyl)sulfonyloxy]-5,6-dihydropyridine-1(2H)-carboxylate	138647-49-1	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)?**

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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 = non-hazardous to waters (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

#### 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/NDL** - 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

#### Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**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)

## Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

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

**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 .**

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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**