

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

1.1. Product identifier

Product Description: **tert-Butyl 4-(3-hydroxyphenyl)perhydro-1,4-diazepine-1-carboxylate**
Cat No. : **MO07901CB; MO07901DA; MO07901EA; MO07901ZZ**
Molecular Formula **C16 H24 N2 O3**

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 Pharmaceuticaaan 3a
2440 Geel, Belgium

UK entity/business name
Thermo Fisher Scientific (Heysham),
Shore Road,
Port of Heysham Industrial Park,
Heysham, Lancashire, LA3 2XY
United Kingdom

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

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

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

Based on available data, the classification criteria are not met

Health hazards

| | |
|--|-------------------|
| Acute oral toxicity | Category 4 (H302) |
| Acute dermal toxicity | Category 4 (H312) |
| Acute Inhalation Toxicity - Dusts and Mists | Category 4 (H332) |
| 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

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

P301 + P330 + P331 - IF SWALLOWED: rinse mouth. Do NOT induce vomiting
P312 - Call a POISON CENTER or doctor if you feel unwell
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
P337 + P313 - If eye irritation persists: Get medical advice/attention
P280 - Wear protective gloves/protective clothing/eye protection/face protection
P332 + P313 - If skin irritation occurs: Get medical advice/attention

2.3. Other hazards

This product does not contain any known or suspected endocrine disruptors

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

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3.1. Substances

| Component | CAS No | EC No | Weight % | CLP Classification - Regulation (EC) No 1272/2008 |
|---|-------------|-------|----------|--|
| tert-Butyl 4-(3-hydroxyphenyl)perhydro-1,4-diazepine -1-carboxylate | 886851-68-9 | | > 95 | STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Acute Tox. 4 (H302) Acute Tox. 4 (H312) Acute Tox. 4 (H332) |

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 (CO₂). 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

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

Hazardous Combustion Products

Nitrogen oxides (NO_x), Carbon monoxide (CO), Carbon dioxide (CO₂).

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.

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. Store under an inert atmosphere.

Technical Rules for Hazardous Substances (TRGS) 510
Storage Class (LGK) (Germany)

Storage Class/LGK 11

Switzerland - Storage of hazardous substances

Storage class - SC 11/13
<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.

MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

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 adequate ventilation, especially in confined areas. 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)

Hand Protection

Protective gloves

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

Skin and body protection

Long sleeved clothing.

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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 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. 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

Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced
Recommended Filter type: Particulates filter conforming to EN 143

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.

Recommended half mask:- Particle filtering: EN149:2001
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 | Solid | |
| Appearance | Yellow | |
| Odor | No information available | |
| Odor Threshold | No data available | |
| Melting Point/Range | 143 - 144 °C / 289.4 - 291.2 °F | |
| Softening Point | No data available | |
| Boiling Point/Range | No information available | |
| Flammability (liquid) | Not applicable | Solid |
| Flammability (solid,gas) | No information available | |
| Explosion Limits | No data available | |
| Flash Point | No information available | Method - No information available |
| Autoignition Temperature | No data available | |
| Decomposition Temperature | No data available | |
| pH | No data available | |
| Viscosity | Not applicable | Solid |
| Water Solubility | Soluble in water | |
| 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 | Not applicable | Solid |
| Particle characteristics | No data available | |

9.2. Other information

| | |
|-------------------|------------------------|
| Molecular Formula | C16 H24 N2 O3 |
| Molecular Weight | 292.38 |
| Evaporation Rate | Not applicable - Solid |

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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 Reactions

No information available.

None under normal processing.

10.4. Conditions to avoid

Incompatible products.

10.5. Incompatible materials

Acids. Bases. Strong oxidizing agents.

10.6. Hazardous decomposition products

Nitrogen oxides (NO_x). Carbon monoxide (CO). Carbon dioxide (CO₂).

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information

(a) acute toxicity;

Oral

Category 4

Dermal

Category 4

Inhalation

Category 4

(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.

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| | |
|--|--|
| (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 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 | Do not empty into drains. |
|---------------------|---------------------------|

12.2. Persistence and degradability

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

| | |
|---------------------------------|-----------------------------|
| 12.3. Bioaccumulative potential | Bioaccumulation is unlikely |
|---------------------------------|-----------------------------|

12.4. Mobility in soil

The product is water soluble, and may spread in water systems. Will likely be mobile in the 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. |
|-------------------------------------|--|

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| | |
|---------------------------------------|--|
| Contaminated Packaging | Dispose of this container to hazardous or special waste collection point. |
| 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 empty into drains. |
| Switzerland - Waste Ordinance | 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 https://www.fedlex.admin.ch/eli/cc/2015/891/en |

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

| | |
|---|------------------------------|
| 14.1. UN number | UN2811 |
| 14.2. UN proper shipping name | Toxic solid, organic, n.o.s. |
| 14.3. Transport hazard class(es) | 6.1 |
| 14.4. Packing group | III |

ADR

| | |
|---|------------------------------|
| 14.1. UN number | UN2811 |
| 14.2. UN proper shipping name | Toxic solid, organic, n.o.s. |
| 14.3. Transport hazard class(es) | 6.1 |
| 14.4. Packing group | III |

IATA

| | |
|---|------------------------------|
| 14.1. UN number | UN2811 |
| 14.2. UN proper shipping name | Toxic solid, organic, n.o.s. |
| 14.3. Transport hazard class(es) | 6.1 |
| 14.4. Packing group | III |

| | |
|--|----------------------------------|
| 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 |
|--|-------------|--------|--------|-----|-------|------|------|------|------|
| tert-Butyl 4-(3-hydroxyphenyl)perhydro-1,4-diazepine-1-carboxylate | 886851-68-9 | - | - | - | - | - | - | - | - |

| Component | CAS No | TSCA | TSCA Inventory | DSL | NDSL | AICS | NZIoC | PICCS |
|-----------|--------|------|----------------|-----|------|------|-------|-------|
|-----------|--------|------|----------------|-----|------|------|-------|-------|

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| | | | | | | | | |
|---|-------------|---|-----------------------------------|---|---|---|---|---|
| | | | notification - Active-Inactive | | | | | |
| tert-Butyl 4-(3-hydroxyphenyl)perhydro-1,4-d iazepine-1-carboxylate | 886851-68-9 | - | - | - | - | - | - | - |

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-(3-hydroxyphenyl)perhydro-1,4-di azepine-1-carboxylate | 886851-68-9 | - | - | - |

| 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-(3-hydroxyphenyl)perhydro -1,4-diazepine-1-carboxylate | 886851-68-9 | 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

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

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

H302 - Harmful if swallowed
H312 - Harmful in contact with skin
H332 - Harmful if inhaled
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 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.

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

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).

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

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End of Safety Data Sheet