

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

1.1. Product identifier

Product Description: Smoothened Agonist dihydrochloride dihydrate
Cat No. : **J64726**
CAS No 364590-63-6
Molecular Formula C₂₈ H₂₈ Cl N₃ OS.2HCl.2H₂ O

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

Thermo Fisher (Kandel) GmbH
Erlenbachweg 2, 76870 Kandel, Germany
Tel: +49 (0) 721 84007 280
Fax: +49 (0) 721 84007 300

Swiss distributor - Fisher Scientific AG
Neuhofstrasse 11, CH 4153 Reinach
Tel: +41 (0) 56 618 41 11
<https://www.fishersci.ch/ch/en/customer-help-support/forms/email-us.html>

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

CLP Classification - Regulation (EC) No 1272/2008

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Physical hazards

Based on available data, the classification criteria are not met

Health hazards

Based on available data, the classification criteria are not met

Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements

None required

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 |
|--|-------------|-------|----------|---|
| Benzo[b]thiophene-2-carboxamide, 3-chloro-N-[4-(methylamino)cyclohexyl]-N-[[3-(4-pyridinyl)phenyl]methyl]- | 364590-63-6 | | <=100 | - |

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

| | |
|---|---|
| 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. Get medical attention immediately if symptoms occur. |
| Ingestion | Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur. |
| Inhalation | Remove to fresh air. Get medical attention immediately if symptoms occur. |
| Self-Protection of the First Aider | No special precautions required. |

4.2. Most important symptoms and effects, both acute and delayed

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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

Carbon dioxide (CO₂). Powder. Water spray. In case of major fire and large quantities: Evacuate area. Fight fire remotely due to the risk of explosion.

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 (CO₂), Nitrogen oxides (NO_x), Sulfur oxides, Hydrogen chloride.

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. Avoid dust formation.

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. Avoid contact with skin, eyes or 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.

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7.2. Conditions for safe storage, including any incompatibilities

Keep refrigerated. Store under an inert atmosphere. Keep container tightly closed in a dry and well-ventilated place. Protect from moisture.

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

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

None under normal use conditions.

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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 |
|----------------|-------------------|-----------------|-------------|-----------------------|
| Nitrile rubber | See manufacturers | - | EN 374 | (minimum requirement) |
| Neoprene | recommendations | | | |
| Natural rubber | | | | |
| PVC | | | | |

Skin and body protection

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 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

No protective equipment is needed under normal use conditions.

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: Particle filter

Small scale/Laboratory use

Maintain adequate ventilation

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

Odor

No information available

Odor Threshold

No data available

Melting Point/Range

No data available

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 information available

Viscosity

Not applicable

Solid

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

Not applicable

Solid

Particle characteristics

No data available

9.2. Other information

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| | |
|-------------------|-----------------------------|
| Molecular Formula | C28 H28 Cl N3 OS.2HCl.2H2 O |
| Molecular Weight | 599.00 |
| Evaporation Rate | Not applicable - Solid |

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity None known, based on information available

10.2. Chemical stability Light sensitive. Hygroscopic.

10.3. Possibility of hazardous reactions

| | |
|--------------------------|-------------------------------|
| Hazardous Polymerization | No information available. |
| Hazardous Reactions | None under normal processing. |

10.4. Conditions to avoid Exposure to moist air or water.

10.5. Incompatible materials Oxidizing agent.

10.6. Hazardous decomposition products Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NO_x). Sulfur oxides. Hydrogen chloride.

SECTION 11: TOXICOLOGICAL INFORMATION

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

Product Information

| | |
|---------------------|-------------------|
| (a) acute toxicity; | |
| 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

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| | |
|--|---------------------------|
| (h) STOT-single exposure; | No data available |
| (i) STOT-repeated exposure; | No data available |
| Target Organs | No information available. |
| (j) aspiration hazard; | Not applicable Solid |
| 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. |
|---------------------|---|

| | |
|--|--------------------------|
| <u>12.2. Persistence and degradability</u> | No information available |
|--|--------------------------|

| | |
|--|--------------------------|
| <u>12.3. Bioaccumulative potential</u> | No information available |
|--|--------------------------|

| | |
|-------------------------------|--------------------------|
| <u>12.4. Mobility in soil</u> | No information available |
|-------------------------------|--------------------------|

| | |
|---|-----------------------------------|
| <u>12.5. Results of PBT and vPvB assessment</u> | 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

13.1. Waste treatment methods

| | |
|-------------------------------------|---|
| Waste from Residues/Unused Products | 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. |
| Contaminated Packaging | Empty remaining contents. Dispose of in accordance with local regulations. Do not re-use empty containers. |

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| | |
|---------------------------------------|--|
| 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. |
| 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 Not regulated

14.1. UN number
14.2. UN proper shipping name
14.3. Transport hazard class(es)
14.4. Packing group

ADR Not regulated

14.1. UN number
14.2. UN proper shipping name
14.3. Transport hazard class(es)
14.4. Packing group

IATA Not regulated

14.1. UN number
14.2. UN proper shipping name
14.3. Transport hazard class(es)
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 |
|---|-------------|--------|--------|-----|-------|------|------|------|------|
| Benzo[b]thiophene-2-carboxamide | 364590-63-6 | - | - | - | - | X | - | - | - |
| 3-chloro-N-[4-(methylamino)cyclohexyl]-N-[[3-(4-pyridinyl)phenyl]methyl]- | | | | | | | | | |

| Component | CAS No | TSCA | TSCA Inventory notification - Active-Inactive | DSL | NDSL | AICS | NZIoC | PICCS |
|---------------------------------|-------------|------|---|-----|------|------|-------|-------|
| Benzo[b]thiophene-2-carboxamide | 364590-63-6 | - | - | - | - | - | - | - |

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| | | | | | | | | |
|---|--|--|--|--|--|--|--|--|
| 3-chloro-N-[4-(methylamino)cyclohexyl]-N-[[3-(4-pyridinyl)phenyl]methyl]- | | | | | | | | |
|---|--|--|--|--|--|--|--|--|

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) |
|--|-------------|---|---|---|
| Benzo[b]thiophene-2-carboxamide, 3-chloro-N-[4-(methylamino)cyclohexyl]-N-[[3-(4-pyridinyl)phenyl]methyl]- | 364590-63-6 | - | - | - |

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 |
|--|-------------|---|--|
| Benzo[b]thiophene-2-carboxamide, 3-chloro-N-[4-(methylamino)cyclohexyl]-N-[[3-(4-pyridinyl)phenyl]methyl]- | 364590-63-6 | 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

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.

Prepared By

Health, Safety and Environmental Department

Revision Date

13-Mar-2024

Revision Summary

New emergency telephone response service provider.

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

End of Safety Data Sheet