

1 Identification

Product identifier

Product name: Smoothened Agonist dihydrochloride dihydrate

Stock number: J64726

CAS Number:
364590-63-6

Details of the supplier of the safety data sheet

Manufacturer/Supplier:

Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757
Email: tech@alfa.com
www.alfa.com

Information Department: Health, Safety and Environmental Department

Emergency telephone number:

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660. After normal business hours, call Carechem 24 at (866) 928-0789.

2 Hazard(s) identification

Classification of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)

The substance is not classified as hazardous according to 29 CFR 1910 (OSHA HCS).

Hazards not otherwise classified No information known.

Label elements

GHS label elements Not applicable

Hazard pictograms Not applicable

Signal word Not applicable

Hazard statements Not applicable

WHMIS classification Not controlled

Classification system

HMIS ratings (scale 0-4)

(Hazardous Materials Identification System)

HEALTH	1	Health (acute effects) = 1
FIRE	1	Flammability = 1
REACTIVITY	1	Physical Hazard = 1

Other hazards

Results of PBT and vPvB assessment

PBT: Not applicable.

vPvB: Not applicable.

3 Composition/information on ingredients

Chemical characterization: Substances

CAS# Description:

364590-63-6 N-Methyl-N'-(3-pyridinylbenzyl)-N'-(3-chlorobenzo[b]thiophene-2-carbonyl)-1,4-diaminocyclohexane dihydrochloride dihydrate

Concentration: ≤100%

4 First-aid measures

Description of first aid measures

After inhalation

Supply fresh air. If required, provide artificial respiration. Keep patient warm.

Seek immediate medical advice.

After skin contact

Immediately wash with water and soap and rinse thoroughly.

Seek immediate medical advice.

After eye contact Rinse opened eye for several minutes under running water. Then consult a doctor.

After swallowing Seek medical treatment.

Information for doctor

Most important symptoms and effects, both acute and delayed No further relevant information available.

Indication of any immediate medical attention and special treatment needed No further relevant information available.

5 Fire-fighting measures

Extinguishing media

Suitable extinguishing agents Carbon dioxide, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

Special hazards arising from the substance or mixture

If this product is involved in a fire, the following can be released:

Carbon monoxide and carbon dioxide

Sulfur oxides (SOx)

Nitrogen oxides (NOx)

Hydrogen chloride (HCl)

Advice for firefighters

Protective equipment:

Wear self-contained respirator.

Wear fully protective impervious suit.

6 Accidental release measures

Personal precautions, protective equipment and emergency procedures

Wear protective equipment. Keep unprotected persons away.

Ensure adequate ventilation

Environmental precautions: Do not allow material to be released to the environment without proper governmental permits.

Methods and material for containment and cleaning up: Pick up mechanically.

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Prevention of secondary hazards: No special measures required.
Reference to other sections
See Section 7 for information on safe handling
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.
Protective Action Criteria for Chemicals
PAC-1: Substance is not listed.
PAC-2: Substance is not listed.
PAC-3: Substance is not listed.

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7 Handling and storage

Handling
Precautions for safe handling
Handle under dry protective gas.
Keep container tightly sealed.
Information about protection against explosions and fires: No information known.
Conditions for safe storage, including any incompatibilities
Storage
Requirements to be met by storerooms and receptacles: Refrigerate
Information about storage in one common storage facility:
Store in the dark.
Protect from heat.
Store away from water/moisture.
Store away from oxidizing agents.
Further information about storage conditions:
Store under dry inert gas.
This product is hygroscopic.
Keep container tightly sealed.
Protect from humidity and water.
Protect from exposure to light.
Refrigerate
Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection

Additional information about design of technical systems:
Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.
Control parameters
Components with limit values that require monitoring at the workplace:
The product does not contain any relevant quantities of materials with critical values that have to be monitored at the workplace.
Additional information: No data
Exposure controls
Personal protective equipment
General protective and hygienic measures
The usual precautionary measures for handling chemicals should be followed.
Keep away from foodstuffs, beverages and feed.
Remove all soiled and contaminated clothing immediately.
Wash hands before breaks and at the end of work.
Maintain an ergonomically appropriate working environment.
Breathing equipment:
Use suitable respirator when high concentrations are present.
Use suitable respiratory protective device in case of insufficient ventilation.
Recommended filter device for short term use:
Use a respirator with type N95 (USA) or PE (EN 143) cartridges as a backup to engineering controls. Risk assessment should be performed to determine if air-purifying respirators are appropriate. Only use equipment tested and approved under appropriate government standards.
Protection of hands:
Impervious gloves
Check protective gloves prior to each use for their proper condition.
The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.
Penetration time of glove material (in minutes) Not determined
Eye protection: Safety glasses with side shields / NIOSH (US) or EN 166(EU)
Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties
General Information
Appearance:
Form: Solid
Odor: Not determined
Odor threshold: Not determined.
pH-value: Not applicable.
Change in condition
Melting point/Melting range: Not determined
Boiling point/Boiling range: Not determined
Sublimation temperature / start: Not determined
Flammability (solid, gaseous) Not determined.
Ignition temperature: Not determined
Decomposition temperature: Not determined
Auto igniting: Not determined.
Danger of explosion: Not determined.
Explosion limits:
Lower: Not determined
Upper: Not determined
Vapor pressure: Not applicable.
Density: Not determined
Relative density Not determined.
Vapor density Not applicable.
Evaporation rate Not applicable.

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USA

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Solubility in / Miscibility with Water: Partition coefficient (n-octanol/water): Viscosity: dynamic: kinematic: Other information	 Not determined Not determined. Not applicable. Not applicable. No further relevant information available.

10 Stability and reactivity Reactivity No information known. Chemical stability Stable under recommended storage conditions. Thermal decomposition / conditions to be avoided: Decomposition will not occur if used and stored according to specifications. Possibility of hazardous reactions Reacts with strong oxidizing agents Conditions to avoid No further relevant information available. Incompatible materials: Water/moisture Oxidizing agents Heat Light Hazardous decomposition products: Carbon monoxide and carbon dioxide Sulfur oxides (SOx) Nitrogen oxides Hydrogen chloride (HCl)
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11 Toxicological information Information on toxicological effects Acute toxicity: No effects known. LD/LC50 values that are relevant for classification: No data Skin irritation or corrosion: May cause irritation Eye irritation or corrosion: May cause irritation Sensitization: No sensitizing effects known. Germ cell mutagenicity: No effects known. Carcinogenicity: No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH. Reproductive toxicity: No effects known. Specific target organ system toxicity - repeated exposure: No effects known. Specific target organ system toxicity - single exposure: No effects known. Aspiration hazard: No effects known. Subacute to chronic toxicity: No effects known. Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.
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12 Ecological information Toxicity Aquatic toxicity: No further relevant information available. Persistence and degradability No further relevant information available. Bioaccumulative potential No further relevant information available. Mobility in soil No further relevant information available. Additional ecological information: General notes: Do not allow material to be released to the environment without proper governmental permits. Do not allow undiluted product or large quantities to reach ground water, water course or sewage system. Avoid transfer into the environment. Results of PBT and vPvB assessment PBT: Not applicable. vPvB: Not applicable. Other adverse effects No further relevant information available.

13 Disposal considerations Waste treatment methods Recommendation Consult state, local or national regulations to ensure proper disposal. Uncleaned packagings: Recommendation: Disposal must be made according to official regulations.

14 Transport information	
UN-Number DOT, ADN, IMDG, IATA	Not applicable
UN proper shipping name DOT, ADR, ADN, IMDG, IATA	Not applicable
Transport hazard class(es) DOT, ADR, ADN, IMDG, IATA Class	Not applicable
Packing group DOT, ADR, IMDG, IATA	Not applicable
Environmental hazards: Marine pollutant (IMDG):	No
Special precautions for user	Not applicable.
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information: DOT Marine Pollutant (DOT):	No

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UN "Model Regulation":	Not applicable

15 Regulatory information Safety, health and environmental regulations/legislation specific for the substance or mixture GHS label elements Not applicable Hazard pictograms Not applicable Signal word Not applicable Hazard statements Not applicable National regulations This product is not listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical Substance Inventory. Use of this product is restricted to research and development only. This product must be used by or directly under the supervision of a technically qualified individual as defined by TSCA. This product must not be used for commercial purposes or in formulations for commercial purposes. This product is not listed on the Canadian Domestic Substances List (DSL) or the Canadian Non-Domestic Substances List (NDSL). SARA Section 313 (specific toxic chemical listings) Substance is not listed. California Proposition 65 Prop 65 - Chemicals known to cause cancer Substance is not listed. Prop 65 - Developmental toxicity Substance is not listed. Prop 65 - Developmental toxicity, female Substance is not listed. Prop 65 - Developmental toxicity, male Substance is not listed. Information about limitation of use: For use only by technically qualified individuals. Other regulations, limitations and prohibitive regulations Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006. Substance is not listed. The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed. Substance is not listed. Annex XIV of the REACH Regulations (requiring Authorisation for use) Substance is not listed. Chemical safety assessment: A Chemical Safety Assessment has not been carried out.
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16 Other information Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user. Department issuing SDS: Global Marketing Department Date of preparation/Revision: Print date, revision date and version number are in the header of each page. Abbreviations and acronyms: ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road) IMDG: International Maritime Code for Dangerous Goods DOT: US Department of Transportation IATA: International Air Transport Association CAS: Chemical Abstracts Service (division of the American Chemical Society) HMIS: Hazardous Materials Identification System (USA) WHMIS: Workplace Hazardous Materials Information System (Canada) LC50: Lethal concentration, 50 percent LD50: Lethal dose, 50 percent PBT: Persistent, Bioaccumulative and Toxic SVHC: Substances of Very High Concern vPvB: very Persistent and very Bioaccumulative ACGIH: American Conference of Governmental Industrial Hygienists (USA) OSHA: Occupational Safety and Health Administration (USA) NTP: National Toxicology Program (USA) IARC: International Agency for Research on Cancer EPA: Environmental Protection Agency (USA)
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