



SAFETY DATA SHEET

This safety data sheet was created pursuant to the requirements of: Regulation (EC) No. 1907/2006 and Regulation (EC) No. 1272/2008

Revision Date 22-Feb-2023

Revision Number 3

73412 73414 - SAG

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

1.1. Product identifier

Document Number DX21210

Product Name SAG

Synonyms Smoothened Agonist;
3-chloro-N-[trans-4-(methylamino)cyclohexyl]-N-[[3-(4-pyridinyl)phenyl]methyl]-benzo[b]thio
phene-2-carboxamide;

Pure substance/mixture Substance

Contains 3-chloro-N-[4-(methylamino)cyclohexyl]-N-[(3-pyridin-4-ylphenyl)methyl]-1-benzothiophene-2-carboxamide

Molecular weight 490.1

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

Manufacturer

STEMCELL Technologies SARL

40 Rue des Berges, Miniparc Polytec, Bâtiment Sirocco, 38000 Grenoble, France

+33 (0) 4 76 04 75 30

STEMCELL Technologies Germany GmbH

Stolberger Str. 200, 50933, Köln, Germany

+33 (0) 4 76 04 75 30

STEMCELL Technologies UK Ltd.

Building 7100, Cambridge Research Park, Beach Drive, Waterbeach, Cambridge, UK, CB25 9TL

+33 (0) 4 76 04 75 30

For further information, please contact

1.4. Emergency telephone number

Emergency Telephone No information available

Emergency Telephone - \$45 - (EC)1272/2008

Europe 112

Section 2: HAZARDS IDENTIFICATION



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2.1. Classification of the substance or mixture

Regulation (EC) No 1272/2008

Acute toxicity - Oral	Category 3 - (H301)
Chronic aquatic toxicity	Category 4 - (H413)

2.2. Label elements

Contains 3-chloro-N-[4-(methylamino)cyclohexyl]-N-[(3-pyridin-4-ylphenyl)methyl]-1-benzothiophene-2-carboxamide



Signal word

Danger

Hazard statements

Hazard statements

H301 - Toxic if swallowed

H413 - May cause long lasting harmful effects to aquatic life

Precautionary Statements - EU (§28, 1272/2008)

P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor

Additional information

This product requires tactile warnings if supplied to the general public This product requires child resistant fastenings if supplied to the general public

2.3. Other hazards

No information available

Section 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Synonyms

Chemical name	EC No.	CAS No.	Weight-%	Classification according to Regulation (EC) No. 1272/2008 [CLP]	REACH Registration Number
3-chloro-N-[4-(methylamino)cyclohexyl]-N-[(3-pyridin-4-ylphenyl)methyl]-1-benzothiophene-2-carboxamide	-	912545-86-9	100	Acute Tox. 3 (H301) Aquatic Chronic 4 (H413)	No data available

Full text of H- and EUH-phrases: see section 16



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Section 4: FIRST AID MEASURES

4.1. Description of first aid measures

General advice	Show this safety data sheet to the doctor in attendance.
Inhalation	Remove to fresh air.
Eye contact	Rinse thoroughly with plenty of water for at least 15 minutes, lifting lower and upper eyelids. Consult a physician.
Skin contact	Wash skin with soap and water. In the case of skin irritation or allergic reactions see a physician.
Ingestion	Do NOT induce vomiting. Clean mouth with water and drink afterwards plenty of water. Never give anything by mouth to an unconscious person. Get medical attention.

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

Symptoms	No information available.
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4.3. Indication of any immediate medical attention and special treatment needed

Note to physicians	Treat symptomatically.
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Section 5: FIRE-FIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media	Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.
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Unsuitable Extinguishing Media	No information available.
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5.2. Special hazards arising from the substance or mixture

Specific hazards arising from the chemical	No information available.
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5.3. Advice for firefighters

Special protective equipment for fire-fighters	Firefighters should wear self-contained breathing apparatus and full firefighting turnout gear. Use personal protection equipment.
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Section 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions Ensure adequate ventilation.

For emergency responders Use personal protection recommended in Section 8.

6.2. Environmental precautions

Environmental precautions See Section 12 for additional Ecological Information.

6.3. Methods and material for containment and cleaning up

Methods for containment Prevent further leakage or spillage if safe to do so.

Methods for cleaning up Take up mechanically, placing in appropriate containers for disposal.

Prevention of secondary hazards Clean contaminated objects and areas thoroughly observing environmental regulations.

6.4. Reference to other sections

Reference to other sections See section 8 for more information. See section 13 for more information.

Section 7: HANDLING AND STORAGE

7.1. Precautions for safe handling

Advice on safe handling Ensure adequate ventilation.

General hygiene considerations Handle in accordance with good industrial hygiene and safety practice.

7.2. Conditions for safe storage, including any incompatibilities

Storage Conditions Store in accordance with information listed on the Product Information Sheet (PIS). Keep out of the reach of children.

7.3. Specific end use(s)

Identified Uses

Risk Management Methods (RMM) The information required is contained in this Material Safety Data Sheet.



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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.

Derived No Effect Level (DNEL) No information available.

Predicted No Effect Concentration (PNEC) No information available.

8.2. Exposure controls

Personal protective equipment

Eye/face protection No special protective equipment required.

Skin and body protection No special protective equipment required.

Respiratory protection No protective equipment is needed under normal use conditions. If exposure limits are exceeded or irritation is experienced, ventilation and evacuation may be required.

General hygiene considerations Handle in accordance with good industrial hygiene and safety practice.

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 Crystalline
Color No information available
Odor No data available.
Odor threshold No data available

Property	Values	Remarks • Method
pH	No data available	None known



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Melting point / freezing point	No data available	None known
Boiling point / boiling range	No data available	None known
Flash point	No data available	None known
Evaporation rate	No data available	None known
Flammability (solid, gas)	Product is not flammable.	
Flammability Limit in Air		None known
Upper flammability limit:	No data available	
Lower flammability limit:	No data available	
Vapor pressure	No data available	None known
Vapor density	No data available	None known
Relative density	No data available	None known
Water solubility	No data available	None known
Solubility(ies)	DMF: 20 mg/mL; DMSO: 20 mg/mL; Ethanol: 20 mg/mL; Ethanol:PBS(pH 7.2) (1:1): 0.5 mg/mL	None known
Partition coefficient	No data available	None known
Autoignition temperature	No data available	None known
Decomposition temperature	No data available	None known
Kinematic viscosity	No data available	None known
Dynamic viscosity	No data available	None known
Explosive properties	No information available	
Oxidizing properties	No information available	

9.2. Other information

Softening point	No information available
Molecular weight	490.1
Molecular formula	C ₂₈ H ₂₈ CIN ₃ OS
VOC Content (%)	No information available
Liquid Density	No information available
Bulk density	No information available

Section 10: STABILITY AND REACTIVITY

10.1. Reactivity

Reactivity	No information available.
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10.2. Chemical stability

Stability	Stable under recommended transport or storage conditions.
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Explosion data

Sensitivity to Mechanical Impact None.

Sensitivity to Static Discharge None.



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10.3. Possibility of hazardous reactions

Possibility of hazardous reactions None under normal processing.

10.4. Conditions to avoid

Conditions to avoid None known based on information supplied.

10.5. Incompatible materials

Incompatible materials Strong oxidizing agents.

10.6. Hazardous decomposition products

Hazardous decomposition products Carbon dioxide (CO₂). Carbon monoxide. Hydrogen sulfide. Nitrogen oxides (NO_x). Phosgene.

Section 11: TOXICOLOGICAL INFORMATION

11.1. Information on toxicological effects

Information on likely routes of exposure

Product Information

Inhalation	Specific test data for the substance or mixture is not available.
Eye contact	Specific test data for the substance or mixture is not available.
Skin contact	Specific test data for the substance or mixture is not available.
Ingestion	Specific test data for the substance or mixture is not available. Toxic if swallowed. (based on components).

Symptoms related to the physical, chemical and toxicological characteristics

Symptoms No information available.

Numerical measures of toxicity

Acute toxicity

The following values are calculated based on chapter 3.1 of the GHS document

ATEmix (oral) 100.00 mg/kg

Unknown acute toxicity 100 % of the mixture consists of ingredient(s) of unknown toxicity.



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0 % of the mixture consists of ingredient(s) of unknown acute oral toxicity.
 100 % of the mixture consists of ingredient(s) of unknown acute dermal toxicity.
 100 % of the mixture consists of ingredient(s) of unknown acute inhalation toxicity (gas).
 100 % of the mixture consists of ingredient(s) of unknown acute inhalation toxicity (vapor).
 100 % of the mixture consists of ingredient(s) of unknown acute inhalation toxicity (dust/mist).

Product Information

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Skin corrosion/irritation No information available.

Product Information

Serious eye damage/eye irritation No information available.

Product Information

Respiratory or skin sensitization No information available.

Product Information

Germ cell mutagenicity No information available.

Product Information

Carcinogenicity No information available.

Product Information

Reproductive toxicity No information available.

Product Information

STOT - single exposure No information available.

Product Information

STOT - repeated exposure No information available.

Product Information

Aspiration hazard No information available.

Section 12: ECOLOGICAL INFORMATION

12.1. Toxicity

Ecotoxicity May cause long lasting harmful effects to aquatic life.

Unknown aquatic toxicity Contains 0 % of components with unknown hazards to the aquatic environment.



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Product Information

12.2. Persistence and degradability

Persistence and degradability No information available.

12.3. Bioaccumulative potential

Bioaccumulation No information available.

12.4. Mobility in soil

Mobility in soil No information available.

12.5. Results of PBT and vPvB assessment

PBT and vPvB assessment No information available.

12.6. Other adverse effects

Other adverse effects No information available.

Section 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

Waste from residues/unused products Dispose of in accordance with local regulations. Dispose of waste in accordance with environmental legislation.

Contaminated packaging Do not reuse empty containers.

Section 14: TRANSPORT INFORMATION

Note: When sold in quantities of less than or equal to 1 mL, or 1 g, with an Excepted Quantity Code of E1, E2, E4, or E5, this item meets the De Minimis Quantities exemption, per IATA 2.6.10. Therefore packaging does not have to be labeled as Dangerous Goods/Excepted Quantity.

IMDG

14.1 UN Number UN2811
14.2 UN proper shipping name TOXIC SOLID, ORGANIC, N.O.S. (SAG)
14.3 Transport hazard class(es) 6.1 Toxic substances



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14.4 Packing Group III
14.5 Marine pollutant Not applicable
14.6 Special Provisions None
14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code No information available

RID

14.1 UN Number Not regulated
14.2 UN proper shipping name Not regulated
14.3 Transport hazard class(es) Not regulated
14.4 Packing Group Not regulated
14.5 Environmental hazard Not applicable
14.6 Special Provisions None

ADR

14.1 UN Number Not regulated
14.2 UN proper shipping name Not regulated
14.3 Transport hazard class(es) Not regulated
14.4 Packing Group Not regulated
14.5 Environmental hazard Not applicable
14.6 Special Provisions None

IATA

14.1 UN Number **Not regulated**
14.2 UN proper shipping name UN2811
14.3 Transport hazard class(es) Toxic solid, organic, n.o.s. (SAG)
14.4 Packing Group 6.1 Toxic substances
14.5 Environmental hazard III
14.6 Special Provisions Not applicable
None

Section 15: REGULATORY INFORMATION

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

European Union

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

Authorizations and/or restrictions on use:

This product does not contain substances subject to authorization (Regulation (EC) No. 1907/2006 (REACH), Annex XIV) This product does not contain substances subject to restriction (Regulation (EC) No. 1907/2006 (REACH), Annex XVII)



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Persistent Organic Pollutants

Not applicable

Ozone-depleting substances (ODS) regulation (EC) 1005/2009 Not applicable

International Inventories

TSCA	Does not comply
DSL/NDSL	Does not comply
EINECS/ELINCS	Does not comply
ENCS	Does not comply
IECSC	Does not comply
KECL	Does not comply
PICCS	Does not comply
AICS	Does not comply

Legend:

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory
DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List
EINECS/ELINCS - European Inventory of Existing Chemical Substances/European List of Notified Chemical Substances
ENCS - Japan Existing and New Chemical Substances
IECSC - China Inventory of Existing Chemical Substances
KECL - Korean Existing and Evaluated Chemical Substances
PICCS - Philippines Inventory of Chemicals and Chemical Substances
AICS - Australian Inventory of Chemical Substances

15.2. Chemical safety assessment

Chemical Safety Report No information available

Section 16: OTHER INFORMATION

Key or legend to abbreviations and acronyms used in the safety data sheet

Full text of H-Statements referred to under section 3

H301 - Toxic if swallowed

H413 - May cause long lasting harmful effects to aquatic life

Legend

SVHC: Substances of Very High Concern for Authorization:

Legend Section 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

TWA	TWA (time-weighted average)	STEL	STEL (Short Term Exposure Limit)
Ceiling	Maximum limit value	*	Skin designation



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This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006

Disclaimer

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