



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 02-Nov-2022

Revision Number 1

100-1052 - XAV939

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

1.1. Product identifier

Document Number 10000014807

Product Name XAV939

Synonyms 2-[4-(trifluoromethyl)phenyl]-1,5,7,8-tetrahydrothiopyrano[4,3-d]pyrimidin-4-one

Pure substance/mixture Substance

Contains 2-[4-(trifluoromethyl)phenyl]-3H,4H,5H,7H,8H-thiopyrano[4,3-d]pyrimidin-4-one

Molecular weight 312.3

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

2.1. Classification of the substance or mixture



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Regulation (EC) No 1272/2008

Acute toxicity - Oral	Category 3 - (H301)
Serious eye damage/eye irritation	Category 1 - (H318)

2.2. Label elements

Contains 2-[4-(trifluoromethyl)phenyl]-3H,4H,5H,7H,8H-thiopyrano[4,3-d]pyrimidin-4-one



Signal word

Danger

Hazard statements

Hazard statements

H301 - Toxic if swallowed

H318 - Causes serious eye damage

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

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

P280 - Wear 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

P310 - 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 Substances

Chemical name	EC No.	CAS No.	Weight-%	Classification according to Regulation (EC) No. 1272/2008 [CLP]	REACH Registration Number
2-[4-(trifluoromethyl)phenyl]-3H,4H,5H,7H,8H-thiopyrano[4,3-d]pyrimidin-4-one	-	284028-89-3	100	Acute Toxicity – Oral – Acute Tox. 3 (H301) Eye Dam. 1 (H318)	No data available



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

Section 4: FIRST AID MEASURES

4.1. Description of first aid measures

General advice	Immediate medical attention is required. Show this safety data sheet to the doctor in attendance.
Inhalation	Remove to fresh air. Get medical attention immediately if symptoms occur.
Eye contact	Get immediate medical advice/attention. Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Keep eye wide open while rinsing. Do not rub affected area.
Skin contact	Wash off immediately with soap and plenty of water for at least 15 minutes. Get medical attention if irritation develops and persists.
Ingestion	Clean mouth with water and drink afterwards plenty of water. Never give anything by mouth to an unconscious person. Do NOT induce vomiting. Get medical attention.
Self-protection of the first aider	Avoid contact with skin, eyes or clothing. Wear personal protective clothing (see section 8).

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

Symptoms	Burning sensation.
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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.
Unsuitable Extinguishing Media	No information available.

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.

Section 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions

Avoid contact with skin, eyes or clothing. Use personal protective equipment as required.

Other Information

Refer to protective measures listed in Sections 7 and 8.

For emergency responders

Use personal protection recommended in Section 8.

6.2. Environmental precautions

Environmental precautions

Prevent further leakage or spillage if safe to do so.

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

Handle in accordance with good industrial hygiene and safety practice. Avoid contact with skin, eyes or clothing. Do not eat, drink or smoke when using this product.

General hygiene considerations

Avoid contact with skin, eyes or clothing. Wear suitable gloves and eye/face protection. Do not eat, drink or smoke when using this product.

7.2. Conditions for safe storage, including any incompatibilities

Storage Conditions

Store in accordance with information listed on the Product Information Sheet (PIS).



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7.3. Specific end use(s)

Identified Uses

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

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

Tight sealing safety goggles.

Hand protection

Wear suitable gloves.

Skin and body protection

Wear suitable protective clothing.

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

Avoid contact with skin, eyes or clothing. Wear suitable gloves and eye/face protection. Do not eat, drink or smoke when using this product.

Environmental exposure controls

No information available.

Section 9: PHYSICAL AND CHEMICAL PROPERTIES



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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
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.	None known
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: 5 mg/mL; DMF:PBS (pH 7.2)(1:5): 0.15 mg/mL; DMSO: 2 mg/mL	
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	312.3
Molecular formula	C14H11F3N2OS
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.

Explosion data

Sensitivity to Mechanical Impact None.

Sensitivity to Static Discharge None.

10.3. Possibility of hazardous reactions

Possibility of hazardous reactions None under normal processing.

Hazardous polymerization Hazardous polymerization does not occur.

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 fluoride. Sulfur oxides.

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. Severely irritating to eyes. Causes serious eye damage. May cause burns. May cause irreversible damage to eyes.

Skin contact Specific test data for the substance or mixture is not available. May cause irritation.

Ingestion Ingestion may cause gastrointestinal irritation, nausea, vomiting and diarrhea. 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



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Symptoms Redness. Burning. May cause blindness.

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.

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 May cause skin irritation.

Product Information

Serious eye damage/eye irritation Classification based on data available for ingredients. Causes burns. Risk of serious damage to eyes.

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



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Aspiration hazard No information available.

Section 12: ECOLOGICAL INFORMATION

12.1. Toxicity

Ecotoxicity The environmental impact of this product has not been fully investigated.

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

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.



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Section 14: TRANSPORT INFORMATION

Note:

Transport in accordance with local, state, and federal regulations. 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. (XAV939)
14.3 Transport hazard class(es)	6.1 Toxic substances
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	UN2811
14.2 UN proper shipping name	Toxic solid, organic, n.o.s.(XAV939)
14.3 Transport hazard class(es)	6.1 Toxic substances
Subsidiary hazard class	6.1
14.4 Packing Group	III
14.5 Environmental hazard	Not applicable
14.6 Special Provisions	None

Section 15: REGULATORY INFORMATION

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



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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)

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



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Full text of H-Statements referred to under section 3

H301 - Toxic if swallowed

H318 - Causes serious eye damage

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

Revision Date

02-Nov-2022

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

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. STEMCELL Technologies Inc. shall not be held liable for any damage resulting from handling or from contact with the product.