SAFETY DATA SHEET

This safety data sheet was created pursuant to the requirements of:
US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

Revision Date 28-Aug-2026 **Revision Number** 2

1. Identification

Product identifier

Product Name XAV939

Other means of identification

Catalog Number 100-1052

UN/ID no. UN2811

Document Number 10000014807

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

Recommended use of the chemical and restrictions on use

Recommended Use Laboratory chemicals

Restrictions on use No information available.

Details of the supplier of the safety data sheet

Manufacturer/Supplier
STEMCELL Technologies Inc.
2323 - 222 Third Street
Cambridge, Massachusetts 02142
1 800 667 0322

STEMCELL Technologies Canada Inc.
1618 Station Street
Vancouver, British Columbia V6A 1B6 Canada
1 800 667 0322

STEMCELL Technologies China Co., Ltd. - Shanghai Main Office
Unit 21BCD, Urban City Centre, 45 Nanchang Road, Huangpu District
Shanghai 200020 P.R.China
400 885 9050

STEMCELL Technologies Australia Pty. Ltd.
PO BOX 648
Tullamarine, VIC, 3043, Australia
1 800 060 350

Emergency telephone number

Emergency Telephone 1-800-667-0322

2. Hazard(s) identification

Classification of the substance or mixture

Acute toxicity - Oral	Category 3
Serious eye damage/eye irritation	Category 2A

Hazards not otherwise classified (HNOC)
Not applicable.

Label elements

Danger

Hazard statements
Toxic if swallowed.
Causes serious eye irritation.

Precautionary Statements - Prevention
Wash face, hands and any exposed skin thoroughly after handling.
Do not eat, drink or smoke when using this product.
Wear protective gloves, protective clothing, eye protection, face protection, and hearing protection.

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
If eye irritation persists: Get medical advice/attention.
IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
Rinse mouth.

Precautionary Statements - Storage
Store locked up.

Precautionary Statements - Disposal
Dispose of contents and container in accordance with local, regional, national, and international regulations as applicable.

Hazards classified under paragraph (d)(1)(ii) of 1910.1200
No information available.

Other Information
No information available.

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3. Composition/information on ingredients

Substance

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

Chemical name	CAS No.	Weight-%	Trade secret
2-[4-(trifluoromethyl)phenyl]-3H,4H,5H,7H,8H-thiopyrano[4,3-d]pyrimidin-4-one	284028-89-3	100	*

*The exact percentage (concentration) of composition has been withheld as a trade secret.

4. First-aid measures

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 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. Get medical attention if irritation develops and persists.

Skin contact Wash skin with soap and water.

Ingestion Clean mouth with water and drink afterwards plenty of water. Do NOT induce vomiting. Rinse mouth. Never give anything by mouth to an unconscious person. Get medical attention.

Self-protection of the first aider Avoid contact with skin, eyes or clothing. Wear personal protective clothing (see section 8).

Most important symptoms and effects, both acute and delayed

Symptoms May cause redness and tearing of the eyes. Burning sensation.

Effects of Exposure No information available.

Indication of any immediate medical attention and special treatment needed

Note to physicians Treat symptomatically.

5. Fire-fighting measures

Suitable Extinguishing Media Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

Unsuitable extinguishing media Do not scatter spilled material with high pressure water streams.

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Specific hazards arising from the chemical No information available.

Explosion data

Sensitivity to mechanical impact None.

Sensitivity to static discharge None.

Special protective equipment and precautions for fire-fighters Firefighters should wear self-contained breathing apparatus and full firefighting turnout gear. Use personal protection equipment.

6. Accidental release measures

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.

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 Pick up and transfer to properly labeled containers.

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

7. Handling and storage

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.

Conditions for safe storage, including any incompatibilities

Storage Conditions Store in accordance with information listed on the Product Information Sheet (PIS). Keep containers tightly closed in a dry, cool and well-ventilated place. Keep out of the reach of children.

8. Exposure controls/personal protection

Control Parameters

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Exposure Limits	This product, as supplied, contains materials that do not have reportable occupational exposure limits or are not subject to the reporting requirements of the local jurisdiction.
Biological occupational exposure limits	This product, as supplied, contains materials that do not have reportable biological exposure limits or are not subject to the reporting requirements of the local jurisdiction.

Appropriate engineering controls

Engineering controls	Showers Eyewash stations Ventilation systems.

Individual protection measures, such as personal protective equipment

Eye/face protection	Wear safety glasses with side shields (or 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.

9. Physical and chemical properties

Information on basic physical and chemical properties

Appearance	Crystalline
Physical state	Solid
Color	No information available
Odor (includes odor threshold)	No information available

Property	**Values**	**Remarks • Method**
Melting point / freezing point	No data available	None known
Boiling point (or initial boiling point or boiling range)	No data available	None known
Flammability (solid, gas)	No data available	None known
Flammability Limit in Air		None known
Upper flammability limit:	No data available	
Lower flammability limit:	No data available	
Flash point	No data available	None known
Autoignition temperature	No data available	None known
Decomposition temperature	No data available	None known
SADT (°C)	No data available	None known
pH	No data available	None known
pH (as aqueous solution)	No data available	None known
Kinematic viscosity	No data available	None known
Dynamic viscosity	No data available	None known
Solubility	DMF: 5 mg/mL; DMF:PBS (pH 7.2)(1:5): 0.15	

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	mg/mL; DMSO: 2 mg/mL	
Water solubility	No data available	None known
Partition coefficient n-octanol/water (log value)	No data available	None known
Vapor pressure (includes evaporation rate)	No data available	None known
Evaporation rate	No data available	None known
Density and/or relative density	No data available	None known
Bulk density	No data available	
Liquid Density	No data available	
Vapor density	No data available	None known
Particle characteristics		None known
Particle Size	No data available	
Particle Size Distribution	No data available	

Other information

Molecular formula	C14H11F3N2OS
Molecular weight	312.3
	Product is not flammable.

10. Stability and reactivity

Reactivity No information available.

Chemical stability Stable under normal conditions.

Possibility of hazardous reactions None under normal processing.

Hazardous polymerization Hazardous polymerization does not occur.

Conditions to avoid None known based on information supplied.

Incompatible materials None known based on information supplied.

Hazardous decomposition products Carbon dioxide (CO2). Carbon monoxide. Hydrogen fluoride. Sulfur oxides.

11. Toxicological information

Information on likely routes of exposure

Product Information

Inhalation Specific test data for the substance or mixture is not available. May cause irritation of respiratory tract.

Eye contact Specific test data for the substance or mixture is not available. Causes serious eye irritation. (based on components). May cause redness, itching, and pain.

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

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Ingestion Specific test data for the substance or mixture is not available. Ingestion may cause gastrointestinal irritation, nausea, vomiting and diarrhea. Toxic if swallowed. (based on components).

Symptoms related to the physical, chemical and toxicological characteristics

Symptoms May cause redness and tearing of the eyes. Burning sensation.

Acute toxicity Toxic if swallowed.

Numerical measures of toxicity No information available.

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

Skin corrosion/irritation No information available.

Serious eye damage/eye irritation Classification based on data available for ingredients. Causes serious eye irritation.

Respiratory or skin sensitization No information available.

Germ cell mutagenicity No information available.

Carcinogenicity No information available.

Reproductive toxicity No information available.

STOT - single exposure No information available.

STOT - repeated exposure No information available.

Aspiration hazard No information available.

Other adverse effects No information available.

Interactive effects No information available.

12. Ecological information

Ecotoxicity Avoid release into the environment.

Persistence and degradability No information available.

Bioaccumulative potential No information available.

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Mobility in soil No information available.

Other adverse effects No information available.

13. Disposal considerations

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.

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.

DOT

UN/ID no.	UN2811
Proper shipping name	Toxic solid, organic, n.o.s.(XAV939)
Hazard class	6.1 Toxic substances
Packing Group	III

TDG Not regulated

MEX Not regulated

ICAO (air) Not regulated

IATA

UN number or ID number	UN2811
UN proper shipping name	Toxic solid, organic, n.o.s.(XAV939)
Transport hazard class(es)	6.1 Toxic substances
Subsidiary hazard class	6.1
Packing Group	III

IMDG

UN number or ID number	UN2811
UN proper shipping name	TOXIC SOLID, ORGANIC, N.O.S. (XAV939)
Transport hazard class(es)	6.1 Toxic substances
Packing Group	III

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15. Regulatory information

International Regulations

The Montreal Protocol on Substances that Deplete the Ozone Layer Not applicable

The Stockholm Convention on Persistent Organic Pollutants Not applicable

The Rotterdam Convention Not applicable

International Inventories

TSCA	Contact supplier for inventory compliance status.
DSL/NDSL	Contact supplier for inventory compliance status.
EINECS/ELINCS	Contact supplier for inventory compliance status.
ENCS	Contact supplier for inventory compliance status.
IECSC	Contact supplier for inventory compliance status.
KECL	Contact supplier for inventory compliance status.
PICCS	Contact supplier for inventory compliance status.
AIIC	Contact supplier for inventory compliance status.
NZIoC	Contact supplier for inventory compliance status.
TCSI	Contact supplier for inventory compliance status.

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
AIIC - Australian Inventory of Industrial Chemicals
NZIoC - New Zealand Inventory of Chemicals
TCSI - Taiwan Chemical Substance Inventory

US Federal Regulations

SARA 313
Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372.

SARA 311/312 Hazard Categories
Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act)
This product does not contain any substances regulated as pollutants pursuant to the Clean Water Act (40 CFR 122.21 and 40 CFR 122.42).

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CAA (Clean Air Act)
This product does not contain any substances regulated as pollutants pursuant to Clean Air Act (CAA).

CERCLA
This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

US State Regulations

California Proposition 65
This product does not contain any Proposition 65 chemicals

U.S. State Right-to-Know Regulations
This product does not contain any substances regulated under applicable state right-to-know regulations

U.S. EPA Label Information

EPA Pesticide Registration Number Not applicable

16. Other information

NFPA	**Health hazards** 2	**Flammability** 0	**Instability** 0	**Special hazards** -
HMIS	**Health hazards** 2	**Flammability** 0	**Physical hazards** 0	**Personal protection** -

Key or legend to abbreviations and acronyms used in the safety data sheet
List may include phrases which are not applicable to this product

ACGIH	American Conference of Governmental Industrial Hygienists
ADN	Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways (Europe)
ADR	Agreement concerning the International Carriage of Dangerous Goods by Road (Europe)
AIIC	Australian Inventory of Industrial Chemicals
ATE	Acute Toxicity Estimate
ASTM	American Society for the Testing of Materials
bar	Biological Reference Values for Chemical Compounds in the Work Area
BAT	Biological tolerance values for occupational exposure
BEL	Biological exposure limits
bw	Body weight
Ceiling	Maximum limit value
CMR	Carcinogen, Mutagen or Reproductive Toxicant
DOT	Department of Transportation (United States)
DSL	Domestic Substances List (Canada)
EmS	Emergency Schedule
ENCS	Existing and New Chemical Substances (Japan)
EPA	U.S. Environmental Protection Agency

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GHS	Globally Harmonized System
HMIS	Hazardous Materials Identification System
IARC	International Agency for Research on Cancer
IATA	International Air Transport Association
IBC	International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk
ICAO	International Civil Aviation Organization
IECSC	Inventory of Existing Chemical Substances in China
IMDG	International Maritime Dangerous Goods
IMO	International Maritime Organization
ISO	International Organization for Standardization
KECI	Korean Existing Chemicals Inventory
LC50	Lethal Concentration to 50% of a test population
LD50	Lethal Dose to 50% of a test population (Median Lethal Dose)
MARPOL	International Convention for the Prevention of Pollution from Ships
NFPA	National Fire Protection Association
NIOSH	National Institute for Occupational Safety and Health
n.o.s.	Not Otherwise Specified
NOAEC	No Observed Adverse Effect Concentration
NOAEL	No Observed Adverse Effect Level
NOELR	No Observable Effect Loading Rate
NTP	National Toxicology Program (United States)
NZIoC	New Zealand Inventory of Chemicals
OECD	Organization for Economic Cooperation and Development
OEL	Occupational exposure limits
OSHA	Occupational Safety and Health Administration of the US Department of Labor
PBT	Persistent, Bioaccumulative and Toxic substance
PICCS	Philippines Inventory of Chemicals and Chemical Substances
PMT	Persistent, Mobile and Toxic
PPE	Personal protective equipment
QSAR	Quantitative Structure Activity Relationship
RID	Agreement concerning the International Carriage of Dangerous Goods by Rail (Europe)
SADT	Self-Accelerating Decomposition Temperature
SAR	Structure-activity relationship
SARA	Superfund Amendments and Reauthorization Act
SDS	Safety Data Sheet
SL	Surface Limit
STEL	Short Term Exposure Limit
STOT RE	Specific target organ toxicity - Repeated exposure
STOT SE	Specific target organ toxicity - Single exposure
TCSI	Taiwan Chemical Substance Inventory
TDG	Transport of Dangerous Goods (Canada)
TSCA	Toxic Substances Control Act (United States)
TWA	Time-Weighted Average
UN	United Nations
VOC	Volatile organic compounds
vPvB	Very Persistent and Very Bioaccumulative
vPvM	Very Persistent and Very Mobile
As	Allergenic substance
DS	Dermal Sensitizer

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Ot	Ototoxicant
pOt	Ototoxicant - potential to cause hearing disorders
PS	Photosensitizer
RS	Respiratory Sensitizer
S	Sensitizer
poS	Sensitizer - capable of causing occupational asthma
Sa	Simple asphyxiant
Sd	Skin designation
pSd	Skin designation - potential for cutaneous absorption
Sdv	Skin designation - vacated
Sk	Skin notation
dSk	Skin notation - danger of cutaneous absorption
pSk	Skin notation - potential for cutaneous absorption

Key literature references and sources for data used to compile the SDS
U.S. Agency for Toxic Substances and Disease Registry (ATSDR)
U.S. Environmental Protection Agency ChemView Database
European Food Safety Authority (EFSA)
U.S. Environmental Protection Agency
Acute Exposure Guideline Level(s) (AEGL(s))
U.S. Environmental Protection Agency Federal Insecticide, Fungicide, and Rodenticide Act
U.S. Environmental Protection Agency High Production Volume Chemicals
Food Research Journal
Hazardous Substance Database
International Uniform Chemical Information Database (IUCLID)
Japan National Institute of Technology and Evaluation (NITE)
Australia National Industrial Chemicals Notification and Assessment Scheme (NICNAS)
NIOSH (National Institute for Occupational Safety and Health)
National Library of Medicine's ChemID Plus (NLM CIP)
National Library of Medicine’s PubMed database (NLM PUBMED)
U.S. National Toxicology Program (NTP)
New Zealand's Chemical Classification and Information Database (CCID)
International Organization for Economic Co-operation and Development (OECD) Environment, Health, and Safety Publications
International Organization for Economic Co-operation and Development (OECD) High Production Volume Chemicals Program
International Organization for Economic Co-operation and Development (OECD) Screening Information Data Set
United Nations World Health Organization (WHO)

Revision Date 28-Aug-2026
Revision Note No information available.

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

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