

XAV-939 SDS | MSDS

1.PRODUCT AND COMPANY IDENTIFICATION

Product identifier

- **Product Name:** XAV-939
- **Catalog Number:** S1180
- **CAS Number:** 284028-89-3
- **IUPAC Name:** 4H-Thiopyrano[4,3-d]pyrimidin-4-one, 3,5,7,8-tetrahydro-2-[4- (trifluoromethyl)phenyl]-

Relevant identified uses and uses advised against

- **Identified uses:** For research and development use only; laboratory chemicals; manufacture of substances.
- **Uses advised against:** Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

- **Company :** Selleck Chemicals
- **TollFree :** +1 877 796-6397
- **Tel :** +1 832 582-8158
- **Fax :** +1 832 582-8590

Emergency telephone number

- **Emergency phone #:** +1 832 582-8158

2. HAZARDS IDENTIFICATION

GHS Classification

Acute toxicity, Oral (Category 4)

Pictogram:



Signal Word: Warning

Hazard Statements

H302: Harmful if swallowed.

Precautionary Statements

- **Prevention:**
 - P264: Wash skin thoroughly after handling.
 - P270: Do not eat, drink or smoke when using this product.

• **Response:**

• P301 + P312 + P330: IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell. Rinse mouth.

• **Disposal:**

• P501: Dispose of contents/container to an approved waste disposal plant.

Other Hazards

None known.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance/Mixture: Substance

CAS-No.: 284028-89-3

Components

• **Chemical Name:** 4H-Thiopyrano[4,3-d]pyrimidin-4-one, 3,5,7,8-tetrahydro-2-[4- (trifluoromethyl)phenyl]-

• **CAS-No.:** 284028-89-3

• **Concentration:** >= 90 - <= 100%

4. FIRST AID MEASURES

General Advice: Show this safety data sheet to the doctor in attendance.

If Inhaled: After inhalation, move person to fresh air.

In Case of Skin Contact: Take off immediately all contaminated clothing. Rinse skin with water/shower.

In Case of Eye Contact: After eye contact, rinse out with plenty of water. Remove contact lenses.

If Swallowed: After swallowing, immediately make victim drink water (two glasses at most). Consult a physician.

Most Important Symptoms and Effects, Both Acute and Delayed: The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11.

Protection of First-Aiders: For personal protection see section 8.

Notes to Physician: N/A.

5. FIREFIGHTING MEASURES

Suitable Extinguishing Media: Water, Foam, Carbon dioxide (CO₂), Dry powder.

Unsuitable Extinguishing Media: For this substance/mixture, no limitations of extinguishing agents are given.

Specific Hazards During Firefighting: Combustible. Development of hazardous combustion gases or vapors is possible in the event of fire.

Hazardous Combustion Products: Carbon oxides, Nitrogen oxides (NO_x), Sulphur oxides, Hydrogen fluoride.

Specific Extinguishing Methods: N/A.

Further Information: Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special Protective Equipment for Firefighters: In the event of fire, wear self-contained breathing apparatus.

6. ACCIDENTAL RELEASE MEASURES

Personal Precautions, Protective Equipment and Emergency Procedures:

- **Advice for non-emergency personnel:** Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, and consult an expert.
- **Advice for emergency responders:** For personal protection see section 8.

Environmental Precautions: Do not let product enter drains.

Methods and Materials for Containment and Cleaning Up: Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

7. HANDLING AND STORAGE

Precautions for Safe Handling: For precautions see section 2.

Conditions for Safe Storage: Keep container tightly closed in a dry place.

Storage Class: 11, Combustible Solids.

Recommended Storage Temperature: Recommended storage temperature see product label.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Control Parameters: Contains no substances with occupational exposure limit values.

Engineering Measures: N/A.

Personal Protective Equipment:

- **Respiratory Protection:** Required when dusts are generated. Recommended filter type: P2.
- **Hand Protection:** Handle with impervious gloves (Nitrile rubber). Full and splash contact: 0.11 mm thickness, 480 min breakthrough time.
- **Eye Protection:** Use safety glasses tested and approved under appropriate government standards such as NIOSH (US) or EN 166 (EU).
- **Skin and Body Protection:** Protective clothing.
- **Hygiene Measures:** Change contaminated clothing. Preventive skin protection is recommended. Wash hands after working with substance.

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance: powder

Color: white, beige

Odor: N/A

Odor Threshold: N/A

pH: N/A

Melting Point: ca. 404.85 °F / 207.14 °C

Boiling Point/Boiling Range: N/A

Flash Point: Not applicable

Evaporation Rate: N/A

Flammability (solid, gas): N/A

Upper/Lower Flammability or Explosive Limits: N/A

Vapor Pressure: N/A

Relative Vapor Density: N/A

Relative Density: N/A

Density: ca. 1.5 g/cm³ (68 °F / 20 °C)

Water Solubility: N/A

Partition Coefficient (n-octanol/water): log Pow: ca. 2.7 (Bioaccumulation is not expected)

Autoignition Temperature: N/A

Decomposition Temperature: N/A

Viscosity: N/A

Explosive Properties: N/A

Oxidizing Properties: none

Molecular Weight: 312.31 g/mol

10. STABILITY AND REACTIVITY

Reactivity: Flammable organic substances and mixtures in fine distribution may generally have dust explosion potential when whirled up.

Chemical Stability: The product is chemically stable under standard ambient conditions (room temperature).

Possibility of Hazardous Reactions: Violent reactions possible with strong oxidizing agents.

Conditions to Avoid: No information available.

Incompatible Materials: Strong oxidizing agents.

Hazardous Decomposition Products: In the event of fire: see section 5.

11. TOXICOLOGICAL INFORMATION

11.1 Information on Toxicological Effects

- **Acute Toxicity:** Acute toxicity estimate Oral - 500.1 mg/kg (Expert judgement). Inhalation and Dermal: N/A.
- **Skin Corrosion/Irritation:** N/A.
- **Serious Eye Damage/Eye Irritation:** N/A.
- **Respiratory or Skin Sensitization:** N/A.

- **Germ Cell Mutagenicity:** N/A.
- **Carcinogenicity:** No component of this product present at levels greater than or equal to 0.1% is identified as a probable, possible, or confirmed human carcinogen by IARC, NTP, or OSHA.
- **Reproductive Toxicity:** N/A.
- **Specific Target Organ Toxicity - Single Exposure:** N/A.
- **Specific Target Organ Toxicity - Repeated Exposure:** N/A.
- **Aspiration Hazard:** N/A.

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

Ecotoxicity: N/A.

Persistence and Degradability: N/A.

Bioaccumulative Potential: Partition coefficient: n-octanol/water log Pow: ca. 2.7. Bioaccumulation is not expected.

Mobility in Soil: N/A.

Other Adverse Effects: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602.

13. DISPOSAL CONSIDERATIONS

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers. Do not mix with other waste. Handle uncleaned containers like the product itself.

14. TRANSPORT INFORMATION

DOT (49 CFR): Not regulated as a dangerous good.

IMDG: Not regulated as a dangerous good.

IATA: Not regulated as a dangerous good.

Transport in Bulk: Not applicable for product as supplied.

Poison Inhalation Hazard: No.

Special Precautions for User: Not classified as dangerous in the meaning of transport regulations.

15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards

Acute Health Hazard

SARA 313

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM I Intermediate or Final VOC's (40 CFR 60.489).

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. Clean Water Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. Clean Water Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations

Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The components of this product are reported in the following inventories:

TSCA: Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

Chemical Name: 4H-Thiopyrano[4,3-d]pyrimidin-4-one, 3,5,7,8-tetrahydro-2-[4- (trifluoromethyl)phenyl]-

16. OTHER INFORMATION

Revision Date: 2026/07/14

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product. Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or contact with the product.