

SAFETY DATA SHEET (SDS)

XAV939

1. Identification

Product Name: XAV939

Product Code: TB75623

CAS No.: 284028-89-3

Molecular Formula: C₁₄H₁₁F₃N₂OS

Molecular Weight: 312.31

Product Use: For Research Use Only (RUO). Laboratory chemical; manufacture of substances.

Uses Advised Against: Any use other than the identified research use.

Distributed by: Trailhead Biosystems Inc.

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SDSs are available at the following website: www.trailbio.com

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2. Hazard(s) Identification

Classification (OSHA HCS 2024, GHS Rev. 7; 29 CFR 1910.1200)

Acute toxicity, oral – Category 3, H301

Serious eye damage/eye irritation – Category 2A, H319

Hazards not otherwise classified (HNOC)

None.

GHS Label Elements

Pictogram:



Signal Word: Danger

Hazard Statements

H301 – Toxic if swallowed.

H319 – Causes serious eye irritation.

Precautionary Statements – Prevention

P264 – Wash hands thoroughly after handling.

P270 – Do not eat, drink, or smoke when using this product.

P280 – Wear protective gloves/protective clothing/eye protection/face protection.

Precautionary Statements – Response

P305+P351+P338 – IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P330 – Rinse mouth.

Precautionary Statements – Storage

P405 – Store locked up.

Precautionary Statements – Disposal

P501 – Dispose of contents/container in accordance with local regulations.

3. Composition/Information on Ingredients

Substance

Chemical Name: XAV939

CAS No.: 284028-89-3

Molecular Formula: C₁₄H₁₁F₃N₂OS

Molecular Weight: 312.31

Single substance supplied at ≥ 98% (as supplied). See Section 2 for hazard classification.

4. First-Aid Measures

Description of first-aid measures

Eye Contact

Remove any contact lenses, locate eye-wash station, and flush eyes immediately with large amounts of water. Separate eyelids with fingers to ensure adequate flushing. Promptly call a physician.

Skin Contact

Rinse skin thoroughly with large amounts of water. Remove contaminated clothing and shoes and call a physician.

Inhalation

Immediately relocate self or casualty to fresh air. If breathing is difficult, give cardiopulmonary resuscitation (CPR). Avoid mouth-to-mouth resuscitation.

Ingestion

Wash out mouth with water; Do NOT induce vomiting; call a physician.

Most important symptoms/effects, acute and delayed

The most important known symptoms and effects are described in the labelling (see Section 2). See Section 2 for hazard classification.

Indication of immediate medical attention and special treatment needed

Treat symptomatically.

5. Fire-Fighting Measures

Suitable Extinguishing Media

Carbon dioxide (CO₂), alcohol-resistant foam, dry chemical powder, or water spray.

Unsuitable Extinguishing Media

None known.

Specific hazards arising from the chemical

During combustion, may emit irritant fumes.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Immediately evacuate personnel to safe areas. Remove undamaged containers from fire area if safe to do so.

6. Accidental Release Measures

Personal precautions, protective equipment, and emergency procedures

Use full personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist, or gas. Ensure adequate ventilation. Keep personnel away from spill/leak. Refer to protective measures listed in Section 8.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Prevent product from entering drains, waterways, or sewer systems. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Methods for Containment	Prevent further leakage or spillage if safe to do so. Remove all sources of ignition.
Methods for Cleaning Up	Absorb spilled material with an inert absorbent (e.g. sand, silica gel, vermiculite) before transferring into an airtight container. Dispose appropriately according to local regulations.

7. Handling and Storage

Precautions for safe handling

Avoid inhalation and contact with eyes and skin. Avoid dust and aerosol formation. Use only in areas with appropriate exhaust ventilation. Wear personal protective equipment.

Conditions for safe storage, including any incompatibilities

Keep container tightly sealed in a cool, well-ventilated area. Keep away from direct sunlight and sources of ignition.

Recommended storage temperature (powder): –20 °C – 3 years; 4 °C – 2 years

Recommended storage temperature (in solvent): –80 °C – 1 year; –20 °C – 6 months

Shipping: Ambient temperature if less than 2 weeks.

8. Exposure Controls/Personal Protection

Control parameters

Exposure Guidelines

This product contains no substances with established occupational exposure limit (OEL) values.

Appropriate engineering controls

Use only under a chemical fume hood ensuring adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation.

Individual protection measures, such as personal protective equipment

Eye/face protection	Safety goggles with side-shields.
Hand protection	Protective (impervious) gloves.

Skin and body protection

Respiratory protection

General Hygiene Considerations

Environmental exposure controls

Impervious clothing.

Suitable respirator where dust, aerosol or fume may be generated.

Handle in accordance with good industrial hygiene and safety practice. Wash hands before and after use. Do not eat, drink, or smoke when using this product.

Avoid discharge into the environment. Keep the product away from drains, water courses, and soil. Clean spillages safely as soon as possible.

9. Physical and Chemical Properties

Appearance: Solid

Odor: No data available

Odor Threshold: No data available

pH: No data available

Melting point/freezing point: No data available

Boiling point/boiling range: No data available

Flash Point: No data available

Evaporation Rate: No data available

Flammability (solid, gas): No data available

Upper/lower flammability or explosive limits: No data available

Vapor Pressure: No data available

Vapor Density: No data available

Relative Density: 1.5g/cm³

Solubility: DMSO: <15 mg/ml (50 mM)

Partition Coefficient (n-octanol/water): No data available

Autoignition temperature: No data available

Decomposition temperature: No data available

Viscosity: No data available

Explosive properties: No data available

Oxidizing properties: No data available

Molecular Weight: 312.31 g/mol

Physical State at 20 °C: Solid

10. Stability and Reactivity

Reactivity

No data available.

Chemical Stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available.

Conditions to avoid

No data available.

Incompatible Materials

Strong acids/alkalis, strong oxidizing/reducing agents.

Hazardous Decomposition Products

Under fire conditions, may decompose and emit toxic fumes.

Other decomposition products – no data available.

11. Toxicological Information

Information on toxicological effects

Acute toxicity (oral)

Classified as Category 3 (H301); see Section 2.

Skin corrosion/irritation

Classified based on available data; see Section 2.

Serious eye damage/irritation

Classified as Category 2A (H319); see Section 2.

Respiratory or skin sensitization

Classified based on available data; see Section 2.

Germ cell mutagenicity

Classified based on available data; see Section 2.

Reproductive Toxicity

Classified based on available data; see Section 2.

STOT – single exposure

Classified based on available data; see Section 2.

STOT – repeated exposure

Classified based on available data; see Section 2.

Aspiration hazard

Classified based on available data; see Section 2.

Carcinogenicity

IARC, ACGIH, NTP, and OSHA: No component of this product present at a level equal to or greater than 0.1% is identified as a probable, possible, or confirmed human carcinogen by these bodies.

Additional information

RTECS No.: Not available. This information is based on current knowledge; the chemical, physical, and toxicological properties have not been completely investigated.

12. Ecological Information

Ecotoxicity

No data available.

Persistence and degradability

No data available.

Bioaccumulative potential

No data available.

Mobility in soil

No data available.

Results of PBT and vPvB assessment

PBT/vPvB assessment unavailable as chemical safety assessment not required or not conducted.

Other adverse effects

No data available.

13. Disposal Considerations

Waste treatment methods

Ensure product is disposed of by licensed waste carriers in accordance with prevailing country, federal, state, and local regulations.

Contaminated packaging

Ensure inner packaging is disposed of by licensed waste carriers. Some outer packaging may be recyclable if not contaminated in accordance with prevailing country, federal, state and local regulations.

14. Transport Information

DOT:

Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S

UN number: 2811

Class: 6.1

Packing group: III

TDG: Not determined

MEX: Not determined

ICAO: Not determined

IATA:

Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S

UN number: 2811

Class: 6.1

Packing group: III

IMDG:

Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S

UN number: 2811

Class: 6.1

Packing group: III

ADR/RID: Not determined

ADN: Not determined

15. Regulatory Information

U.S. Federal Regulations

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313: This material does not contain any chemical components with known CAS numbers above De Minimis reporting levels under SARA Title III, Section 313.

SARA 311/312 Hazards – Acute Health Hazards. Physical Hazards: None known.

US State Regulations

California Proposition 65: This product does not contain any chemicals known to the State of California to cause cancer, birth defects, or other reproductive harm.

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

Pennsylvania Right to Know: No components subject to the Pennsylvania Right to Know Act.

New Jersey Right to Know: No components subject to the New Jersey Right to Know Act.

16. Other Information

Prepared By	Trailhead Biosystems
Preparation Date	2026-08-20
Revision Date	2026-08-20
Revision Note	No information available

Disclaimer: The information provided in this Safety Data Sheet (SDS) is correct to the best of our knowledge. The information given is designed only as guidance for safe handling, use, processing, storage, transportation, disposal, and release and is not to be considered a warranty or quality specification. This product is For Research Use Only and must be handled only by suitably qualified, experienced personnel in appropriately equipped facilities. The burden of safe use of this material rests with the user. 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.

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