1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1 Product identifiers

Product Name: XAV 939
Catalog Number: 3748
CAS Number: 284028-89-3
IUPAC Name: 3,5,7,8-Tetrahydro-2-[4-(trifluoromethyl)phenyl]-4H-thiopyrano[4,3-d]pyrimidin-4-one

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified Uses: Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company: Tocris Bioscience
The Watkins Building, Atlantic Road, Bristol, BS11 9QD, UK
Telephone: + 44 (0)117 916-3333
Fax: + 44 (0)117 916-3344
Internet: www.tocris.com
E-mail address: info@bio-techne.com

1.4 Emergency Telephone number

Emergency Tel: + 44 (0)117 916-3333 (09.00 - 17.00 GMT)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

This substance does not meet the classification criteria of the EC Directives 67/548/EEC, 1999/45/EC or 1272/2008.

2.2 Label elements

The product does not need to be labelled in accordance with EC directives or respective national laws.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product Name: XAV 939
Formula: C_{14}H_{11}F_{3}N_{2}OS
Molecular Weight: 312.31
CAS Number: 284028-89-3

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice
Consult a doctor and show this safety data sheet.

If inhaled
Remove to fresh air and monitor breathing. If breathing becomes difficult, give oxygen. If breathing stops, give artificial respiration. Consult a doctor.

In case of skin contact
Immediately wash skin with copious amounts of soap and water for at least 15 minutes. Remove contaminated clothing and shoes and wash before reuse. Consult a doctor.

In case of eye contact
Flush with copious amounts of water for at least 15 minutes. Consult a doctor.

If swallowed
Rinse mouth with water. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Consult a doctor.

4.2 Most important symptoms and effects, both acute and delayed

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

4.3 Indication of immediate medical attention and special treatment needed

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
In combustion, may emit toxic fumes.

5.3 **Precautions for fire-fighters**
Wear suitable protective clothing to prevent contact with skin and eyes and self-contained breathing apparatus.

6. **ACCIDENTAL RELEASE MEASURES**

6.1 **Personal precautions, protective equipment and emergency procedures**
Do not take action without suitable protective clothing - see section 8 of SDS. Evacuate personnel to safe areas. Ensure adequate ventilation. Avoid breathing vapors, mist, dust or gas.

6.2 **Environmental precautions**
Do not let product enter drains.

6.3 **Methods and materials for containment and cleaning up**
Cover spillage with suitable absorbent material. Sweep up material and place in an appropriate container. Hold all material for appropriate disposal as described under section 13 of SDS.

6.4 **Reference to other sections**
For required PPE see section 8. For disposal see section 13.

7. **HANDLING AND STORAGE**

7.1 **Precautions for safe handling**
Use in a chemical fume hood, with air supplied by an independent system. Avoid inhalation, contact with eyes, skin and clothing. Avoid the formation of dust and aerosols. Use in a well-ventilated area. Keep away from sources of ignition. Avoid prolonged or repeated exposure.

7.2 **Conditions for safe storage, including any incompatibilities**
Store in cool, well-ventilated area. Keep away from direct sunlight. Keep container tightly sealed until ready for use. Recommended storage temperature: Store at RT

7.3 **Specific end uses**
Use in a laboratory fume hood where possible. Refer to employer's COSHH risk assessment.

8. **EXPOSURE CONTROLS/PERSOAL PROTECTION**

8.1 **Control parameters**

**Components with workplace control parameters**
Contains no substances with occupational exposure limit values.

8.2 **Exposure controls**

**Appropriate engineering controls**
Use in a fume hood where applicable. Ensure all engineering measures described under section 7 of SDS are in place. Ensure laboratory is equipped with a safety shower and eye wash station.

**Personal protective equipment**

**Eye/face protection**
Use appropriate safety glasses.

**Skin protection**
Use appropriate chemical resistant gloves (minimum requirement use standard BS EN 374:2003). Gloves should be inspected before use. Wash and dry hands thoroughly after handling.

**Body protection**
Wear appropriate protective clothing.

**Respiratory protection**
If risk assessment indicates necessary, use a suitable respirator.

9. **PHYSICAL AND CHEMICAL PROPERTIES**

9.1 **Information on basic physical and chemical properties**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Appearance</td>
<td>White solid</td>
<td></td>
</tr>
<tr>
<td>Odor</td>
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</tr>
<tr>
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<tr>
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<td>Partition coefficient</td>
</tr>
<tr>
<td>Boiling point / range</td>
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</tr>
<tr>
<td>Flash point</td>
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<td>Decomposition temperature</td>
</tr>
<tr>
<td>Evaporation rate</td>
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<td>Viscosity</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
<td>No data available</td>
<td>Explosive properties</td>
</tr>
<tr>
<td>Upper / lower flammability or explosive limits</td>
<td>No data available</td>
<td>Oxidising properties</td>
</tr>
</tbody>
</table>

9.2 **Other safety information**
10. STABILITY AND REACTIVITY

10.1 Reactivity
Stable under recommended transport or storage conditions.

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
Hazardous reactions will not occur under normal transport or storage conditions. Decomposition may occur on exposure to conditions or materials listed below.

10.4 Conditions to avoid
Heat, moisture.

10.5 Incompatible materials
Strong acids/alkalis, strong oxidising/reducing agents.

10.6 Hazardous decomposition products
In combustion may emit toxic fumes. No known decomposition information.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects
- **Acute Toxicity**
  No data available
- **Skin corrosion/irritation**
  Classification criteria are not met based on available data
- **Serious eye damage/irritation**
  Classification criteria are not met based on available data
- **Respiratory or skin sensitization**
  Classification criteria are not met based on available data
- **Germ cell mutagenicity**
  Classification criteria are not met based on available data
- **Carcinogenicity**
  Classification criteria are not met based on available data
- **Reproductive toxicity**
  Classification criteria are not met based on available data
- **Specific target organ toxicity - single exposure**
  Classification criteria are not met based on available data
- **Specific target organ toxicity - repeated exposure**
  Classification criteria are not met based on available data
- **Aspiration hazard**
  Classification criteria are not met based on available data

**Symptoms / Routes of exposure**
- Inhilation: There may be irritation of the throat with a feeling of tightness in the chest.
- Ingestion: There may be irritation of the throat.
- Skin: There may be mild irritation at the site of contact.
- Eyes: There may be irritation and redness.

**Delayed / Immediate Effects:** No known symptoms.

**Additional Information**
- RTECS No: Not available
- Exposure may cause irritation of eyes, mucous membranes, upper respiratory tract and skin.
- To the best of our knowledge, the chemical, physical and toxicological properties have not been fully investigated

12. ECOLOGICAL INFORMATION

12.1 Toxicity
No data available

12.2 Persistence and degradability
No data available

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available
12.5 Results of PBT and vPvB assessment
No data available

12.6 Other adverse effects
No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Transfer to a suitable container and arrange for collection by specialized disposal company in accordance with National legislation.

Contaminated packaging
Dispose of in a regulated landfill site or other method for hazardous or toxic wastes in accordance with National legislation.

14. TRANSPORT INFORMATION

Classified according to the criteria of the UN Model Regulations as reflected in the IMDG Code, ADR, RID and IATA.

14.1 UN-Number

Does not meet the criteria for classification as hazardous for transport.

14.2 UN proper shipping name

Does not meet the criteria for classification as hazardous for transport.

14.3 Transport hazard class(es)

Does not meet the criteria for classification as hazardous for transport.

14.4 Packaging group

Does not meet the criteria for classification as hazardous for transport.

14.5 Environmental hazards

This product is not classified as environmentally hazardous according to the UN Model Regulations, nor a marine pollutant according to the IMDG Code.

14.6 Special precautions for users

No data available

15. REGULATORY INFORMATION

This safety datasheet complies with the requirements of Regulation (EC) No. 453/2010.

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

No data available

California Proposition 65
Not applicable

15.2 Chemical safety assessment

A Chemical Safety Assessment has not been made for this product.

16. OTHER INFORMATION

Further Information
Copyright © 2019 Tocris Bioscience. This company shall not be held liable for any damage resulting from handling or from contact with the above product. This material must only be handled by suitably qualified experienced scientists in appropriately equipped and authorized facilities. The above information is believed to be correct but does not purport to be all inclusive and should be used as a guide only for experienced personnel. Always consult your safety advisor and follow appropriate local and national safety legislature. The absence of warning must not, under any circumstance, be taken to mean that no hazard exists.

End of safety data sheet