

Safety Data Sheet

SDS created: 15-10-2018



1 - Identification of substance and manufacturer

Axon catalogue ID 1656	CAS number 626221-47-4	Manufacturer's name Axon Medchem BV	Emergency Telephone number +31 (0)50 311 8007
Product name Irestatin 9389	Batch no. 1	Street address Biotech Center UMCG, Hanzeplein 1	Manufacturer's fax number +31 (0)50 3600390
IUPAC name 2-(3-Cyano-4-(trifluoromethyl)-6,7-dihydro-5H-cyclopenta[b]pyridin-2-ylthio)-N-(4-methylthiazol-2-yl)acetamide	Application Inhibitor of the unfolded protein response and endonuclease IRE1	Postal Code 9713 GZ	City Groningen
		Province Groningen	Country of origin The Netherlands
			Manufacturer's email address info@axonmedchem.com
			Manufacturer's website http://www.axonmedchem.com

2 - Hazards identification

Route of entry Eye contact, Inhalation, Digestion	GHS Pictogram	Potential health effects May be harmful by inhalation, ingestion or eye and/or skin absorption. May cause irritation to eye, mucous membranes, upper respiratory system, and/or skin. The toxicological properties of this compound have not been fully tested. For research purposes only.
Symptoms of Exposure No data available		

3 - Information on ingredients

Hazardous ingredient Irestatin 9389	CAS number 626221-47-4	Concentration 99.2%	LD-50 of ingredient No data available
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4 - First Aid Measures

Skin contact Wash with copious amounts of water for at least 15 minutes. Remove contaminated clothing.	Eye contact Rinse with copious amounts of water for at least 15 minutes as a precaution.	Inhalation Transfer victim to an un-effected area and monitor breathing. If breathing becomes difficult administer oxygen. If breathing stops give artificial respiration.	Ingestion Rinse mouth out with copious amounts of water, contact a physician.
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5 - Fire Fighting Measures

Fire fighting instructions Use appropriate extinguishing media appropriate to the surrounding fire conditions. Wear protective clothing to prevent contact with skin, eyes, and respiratory system.	Flammable No data available	Flashpoint (°C) No data available	Hazardous combustion products May emit toxic gasses like carbon monoxide (CO), carbon dioxide (CO ₂), hydrochloric acid (HCl), nitrogen oxide upon thermal decomposition.
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6 - Accidental Release Measures

Leak and spill procedures

Wear appropriate protective clothing. Vacuum or sweep up dry material and dispose in an appropriate container as described under Disposal Conditions. Avoid raising dust. Absorb solutions with finely-powdered liquid-binding material. After removal, ventilate and decontaminate surfaces and equipment with alcohol. Dispose of contaminated materials according to section 13.

7 - Handling and Storage

Handling procedures and equipment

Avoid inhalation, contact with eyes, skin and clothing. Wear appropriate protective clothing. Avoid repeated and/or prolonged exposure. Use in a chemical fume hood, with an independent air supply.

Storage requirements

Store in a properly sealed container under the storage conditions indicated on the label.

8 - Exposure Control / Personal Protection

Exposure limits No data available	Protection of hands/skin Chemical resistant gloves and lab coat	Protection of eyes Appropriate safety glasses	Protection of respiratory system Handle in fume hood. Prevent inhalation
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9 - Physical and chemical properties

Batch molecular formula C ₁₆ H ₁₃ F ₃ N ₄ O ₂ S ₂	Appearance White solid	Chemical purity 99.2%	Solubility in water (mg/mL) 0.0
Batch MW 398.43	Melting point 191.0 - 191.4 °C	Optical purity (ee) N.A.	

10 - Stability and reactivity

Stability Stable under normal handling conditions.	Reactivity May emit toxic gasses like carbon monoxide (CO), carbon dioxide (CO ₂), hydrochloric acid (HCl), nitrogen oxide upon thermal decomposition.	Conditions and materials to avoid Protect from light and heat. Avoid strong oxidizing agents.
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11 - Toxicological information

Toxicity No data available	Carcinogenicity No data available	Mutagenicity No data available	Teratogenicity No data available
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12 - Ecological information

Treat as potentially toxic. Runoff from fire control or dilution with water may cause pollution.

13 - Disposal considerations

Treat as potentially toxic. Dispose in accordance with local, state, and federal regulations.

14 - Transport Information

(US) DOT shipping name No data available	IATA class No data available	Applicable HS class 2942.00.0000	Transportation (Land/Sea/Air) Non-hazardous
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15 - Regulatory Information

Hazardous ingredient Irestatin 9389	CAS number 626221-47-4
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European risk and safety phrases

R48: Danger of serious damage to health by prolonged exposure.

S22 - Do not breathe dust.

S24/S25 - Avoid any inhalation, contact with skin and eyes.

S36/S37/S39 - Wear suitable protective clothing, gloves and eye/face protection.

S26: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

US EPA SARA Title III

Sec.302 (EHS) - No

Sec.302 (EHS) - No

Sec.313 (TRI) - No

Sec.110 - No

US EPA CAA, CWA, TSCA

EPA CAA - No

EPA CWA NPDES - No

EPA TSCA - No

CA PROP 65 - No

16 - Other information

The above information is believed to be accurate and represents the best information currently available to us, but does not purport to be complete.

The absence of warning must not, under any circumstance, be taken to mean that no hazard exists.

For research use only by trained personnel.

CAUTION: SUBSTANCE NOT FULLY TESTED