

# Material Safety Data Sheet

MSDS created: 26-07-2011



## 1 - Identification of substance and manufacturer

<b>Manufacturer's name</b> Axon Medchem BV	<b>Emergency Telephone number</b> +31 (0)50 311 8007	<b>Axon catalogue ID</b> 1379	<b>CAS number</b> 952021-60-2
<b>Street address</b> Biotech Center UMCG, Hanzeplein 1	<b>Manufacturer's website</b> http://www.axonmedchem.com	<b>Product name</b> PF 477736	<b>Batch no.</b> 4
<b>Postal Code</b> 9713 GZ	<b>Country of origin</b> the Netherlands	<b>IUPAC name</b> (R)-2-Amino-2-cyclohexyl-N-[2-(1-methyl-1H-pyrazol-4-yl)-6-oxo-5,6-dihydro-1H-[1,2]diazepino[4,5,6-cd]indol-8-yl]-acetamide	<b>Application</b> Chk1 inhibitor
<b>City / Province</b> Groningen			

## 2 - Information on ingredients

<b>Hazardous ingredient</b> PF 477736	<b>CAS number</b> 952021-60-2	<b>Concentration</b> 98.5%	<b>LD-50 of ingredient</b> No data available
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## 3 - Hazards identification

<b>Route of entry</b> Eye contact, Inhalation, Digestion	<b>Potential health effects</b> 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.
<b>Symptoms of Exposure</b> No data available	

## 4 - First Aid Measures

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

<b>Fire fighting instructions</b> Use extinguishing media appropriate to the surrounding fire conditions. Wear protective clothing to prevent contact with skin, eyes, and respiratory system.	<b>Flammable</b> No data available	<b>Flashpoint (°C)</b> No data available	<b>Hazardous combustion products</b> May emit toxic gasses like carbon monoxide (CO), carbon dioxide (CO <sub>2</sub> ), 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

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

<b>Batch molecular formula</b> C <sub>22</sub> H <sub>25</sub> N <sub>7</sub> O <sub>2</sub>	<b>Appearance</b> Yellow Solid	<b>Chemical purity</b> 98.5%	<b>Solubility in water (mg/mL)</b> 0
<b>Batch MW</b> 419.48	<b>Melting point</b> 249-250 °C	<b>Optical purity (ee)</b> N.A.	

## 10 - Stability and reactivity

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

<b>Toxicity</b> No data available	<b>Carcinogenicity</b> No data available	<b>Mutagenicity</b> No data available	<b>Teratogenicity</b> 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

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

<b>Hazardous ingredient</b> PF 477736	<b>CAS number</b> 952021-60-2	<b>US EPA SARA Title III</b> Sec.302 (EHS) - No Sec.302 (EHS) - No Sec.313 (TRI) - No Sec.110 - No	<b>US EPA CAA, CWA, TSCA</b> EPA CAA - No EPA CWA NPDES - No EPA TSCA - No CA PROP 65 - No
<b>European risk and safety phrases</b> R26/27/28: Very toxic by inhalation, in contact with skin and if swallowed 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			

## 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