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

1.1 Product identifiers
- **Product Name:** CP 945598 hydrochloride
- **Catalog Number:** 4236
- **CAS Number:** 686347-12-6
- **IUPAC Name:** 1-[8-(2-Chlorophenyl)-9-(4-chlorophenyl)-9H-purin-6-yl]-4-(ethylamino)piperidine-4-carboxamide hydrochloride

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
- **Address:** 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:** customerservice@tocris.co.uk

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.

2.3 Other hazards - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances
- **Product Name:** CP 945598 hydrochloride
- **Formula:** C_{25}H_{25}Cl_{2}N_{7}O.HCl
- **CAS Number:** 686347-12-6
- **Molecular Weight:** 546.88

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. Using non-spark tools, sweep up material and place in an appropriate container. Decontaminate spill site with 10% caustic solution and ventilate area until after disposal is complete. 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 +4°C

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

8. **EXPOSURE CONTROLS/PERSONAL 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>
</tr>
</thead>
<tbody>
<tr>
<td>Appearance</td>
<td>White solid</td>
</tr>
<tr>
<td>Odor</td>
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</tr>
<tr>
<td>Odor threshold</td>
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</tr>
<tr>
<td>pH</td>
<td>No data available</td>
</tr>
<tr>
<td>Melting / freezing point</td>
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</tr>
<tr>
<td>Boiling point / range</td>
<td>No data available</td>
</tr>
<tr>
<td>Flash point</td>
<td>No data available</td>
</tr>
<tr>
<td>Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
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</tr>
<tr>
<td>Upper / lower flammability or</td>
<td>No data available</td>
</tr>
<tr>
<td>explosive limits</td>
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</tr>
<tr>
<td>Vapor pressure</td>
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</tr>
<tr>
<td>Vapor density</td>
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</tr>
<tr>
<td>Relative density</td>
<td>No data available</td>
</tr>
<tr>
<td>Solubility(ies)</td>
<td>Soluble to 20 mM in DMSO</td>
</tr>
<tr>
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</tr>
<tr>
<td>Auto-ignition temperature</td>
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</tr>
<tr>
<td>Decomposition temperature</td>
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<tr>
<td>Viscosity</td>
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<tr>
<td>Explosive properties</td>
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</tr>
<tr>
<td>Oxidising properties</td>
<td>No data available</td>
</tr>
</tbody>
</table>

9.2 **Other safety information**
No data available

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
Inhalation: 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
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
May be harmful to the aquatic environment.

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

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

16. OTHER INFORMATION
Further Information
Copyright © 2016 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