1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{17}\text{H}_{22}\text{F}_{2}\text{N}_{4}\text{O}_{3}\text{S}_{2} \)
Batch Molecular Weight: 432.51
Physical Appearance: Yellow solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C

2. ANALYTICAL DATA

TLC: \( R_{f} = 0.5 \) (Dichloromethane:Methanol [9:1])
HPLC: Shows 98.3% purity
\(^1\text{H} \text{NMR:} \) Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>47.21</td>
<td>47.06</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.13</td>
<td>5.04</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>12.95</td>
<td>12.84</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Information

**Product Name:** BI 605906
**Catalog No.:** 5300
**Batch No.:** 1

- **CAS Number:** 960293-88-3
- **IUPAC Name:** 3-Amino-4-(1,1-difluoropropyl)-6-[4-(methylsulfonyl)-1-piperidinyl]thieno[2,3-b]pyridine-2-carboxamide

**Description:**
Selective IKKβ inhibitor (IC50 = 380 nM). Displays no effect on a panel of 100 kinases, except at IGF1 (IC50 = 7.6 μM).

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C17H22F2N4O3S2
- **Batch Molecular Weight:** 432.51
- **Physical Appearance:** Yellow solid

**Minimum Purity:** >98%

**Solubility & Usage Info:**
DMSO to 100 mM

**Stability and Solubility Advice:**
Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

**SOLIDS:** Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

**SOLUTIONS:** We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**References:**