1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( C_{25}H_{25}N_3O_2S \cdot \frac{1}{2}H_2O \)

Batch Molecular Weight: 440.56

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
ethanol to 5 mM

Storage: Store at +4°C

2. ANALYTICAL DATA

TLC: \( R_f = 0.27 \) (Chloroform:Methanol [97:3])

HPLC: Shows 99.0% purity

\(^1\)H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

<table>
<thead>
<tr>
<th>Theoretical</th>
<th>Found</th>
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</thead>
<tbody>
<tr>
<td>68.16</td>
<td>68.31</td>
</tr>
<tr>
<td>5.95</td>
<td>5.83</td>
</tr>
<tr>
<td>9.54</td>
<td>9.54</td>
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</tbody>
</table>
Product Name: NVP 231
CAS Number: 362003-83-6
IUPAC Name: N-[2-(Benzyloxyamino)-6-benzothiazolyl]tricyclo[3.3.1.13,7]decane-1-carboxamide

Description:
Potent, selective and reversible ceramide kinase (CerK) inhibitor (IC$_{50}$ = 12 nM in vitro). Displays selectivity for CerK over sphingosine kinases (IC$_{50}$ $\geq$ 100 μM) and other lipid kinases.

Physical and Chemical Properties:
Batch Molecular Formula: C$_{25}$H$_{23}$N$_{2}$O$_{2}$S·$\frac{1}{2}$H$_{2}$O
Batch Molecular Weight: 440.56
Physical Appearance: Off-white solid
Minimum Purity: >98%

Storage: Store at +4°C

Solubility & Usage Info:
DMSO to 100 mM
ethanol to 5 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: