1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{19}\text{H}_{22}\text{BrNOS} \)

Batch Molecular Weight: 392.35

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM, ethanol to 100 mM

Storage: Store at +4°C

2. ANALYTICAL DATA

TLC: \( R_f = 0.39 \) (Ethyl acetate:Petroleum ether [4:1])

HPLC: Shows 98% 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>58.16</td>
<td>58.23</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.65</td>
<td>5.6</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>3.57</td>
<td>3.73</td>
</tr>
</tbody>
</table>
Product Name: AZ 12216052
CAS Number: 1290628-31-7
IUPAC Name: 2-[[4-(Bromophenyl)methyl]thio]-N-[4-(1-methylpropyl)phenyl]acetamide

Description:
Positive allosteric modulator at mGlu₉ receptors. Exhibits anxiolytic effects in mouse models of anxiety.

Physical and Chemical Properties:
Batch Molecular Formula: C₁₉H₁₂BrNOS
Batch Molecular Weight: 392.35
Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:
DMSO to 100 mM
ethanol 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: