1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{17}\text{H}_{11}\text{BrN}_{2}\text{O}_{2} \)

Batch Molecular Weight: 355.19

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at RT

2. ANALYTICAL DATA

TLC: \( R_f = 0.58 \) (Chloroform:Methanol [9:1])

HPLC: Shows 99.5% 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>57.49</td>
<td>57.73</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>3.12</td>
<td>3.1</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>7.89</td>
<td>7.9</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: 5-BBDH  
CAS Number: 768404-03-1  
IUPAC Name: 5-(3-Bromophenyl)-1,3-dihydro-2H-benzofuro[3,2-e]-1,4-diazepin-2-one

Description: Potent P2X4 receptor antagonist. Blocks P2X4-mediated currents in Chinese hamster ovary cells (IC50 = 0.50 μM).

Physical and Chemical Properties:
Batch Molecular Formula: C17H13BrN2O2
Batch Molecular Weight: 355.19
Physical Appearance: Off White solid
Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

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: