1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{13}\text{H}_8\text{BrNO}_3 \)

Batch Molecular Weight: 306.11

Physical Appearance: Beige solid

Solubility:
- DMSO to 100 mM
- Ethanol to 50 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.4% purity

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

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>51.01</td>
<td>2.63</td>
<td>4.58</td>
</tr>
<tr>
<td>Found</td>
<td>51.25</td>
<td>2.58</td>
<td>4.55</td>
</tr>
</tbody>
</table>
**Product Name:** WAY 200070  
**CAS Number:** 440122-66-7  
**IUPAC Name:** 7-Bromo-2-(4-hydroxyphenyl)-1,3-benzoxazol-5-ol

**Description:**
Selective ERβ receptor agonist that displays 68-fold selectivity over ERα (EC<sub>50</sub> values are 2 and 155 nM for ERβ and ERα respectively). Displays antianxiolytic and antidepressive effects in vivo.

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C<sub>13</sub>H<sub>8</sub>BrNO<sub>3</sub>
- **Batch Molecular Weight:** 306.11
- **Physical Appearance:** Beige solid
- **Minimum Purity:** >98%
- **Batch Molecular Structure:**

![Molecular Structure](image)

**Storage:** Store at RT

**Solubility & Usage Info:**
- DMSO to 100 mM
- Ethanol to 50 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:**