1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( C_{22}H_{27}N_{3}O_{3}S \cdot HCl \cdot \frac{1}{4}H_2O \)

Batch Molecular Weight: 454.49

Physical Appearance: Off-white solid

Solubility:
- Water to 25 mM
- DMSO to 50 mM
- Ethanol to 10 mM

Storage: Desiccate at +4°C

2. ANALYTICAL DATA

HPLC: Shows 97.7% purity

\(^1\)H 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>58.14</td>
<td>58.08</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>6.32</td>
<td>6.18</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>9.25</td>
<td>9.16</td>
</tr>
</tbody>
</table>
Product Name: KC 12291 hydrochloride
Catalog No.: 3251
Batch No.: 1

CAS Number: 181936-98-1
IUPAC Name: 3,4-Dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]benzeneethanamine hydrochloride

Description:
Orally active atypical voltage-gated sodium channel blocker. Inhibits sustained sodium currents (I_{Na,S}) and prevents diastolic contracture in isolated atria in vitro (IC_{50} values are 9.6 and 0.55 - 0.79 μM respectively). Displays anti-ischemic, bradycardic and cardioprotective activity in vivo.

Physical and Chemical Properties:
Batch Molecular Formula: C_{22}H_{27}N_{2}O_{3}S.HCl.1/4H_{2}O
Batch Molecular Weight: 454.49
Physical Appearance: Off-white solid
Minimum Purity: >97%

Storage:
Desiccate at +4°C

Solubility & Usage Info:
water to 25 mM
DMSO to 50 mM
ethanol to 10 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: