1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{18}\text{H}_{31}\text{NO}_{4}.\frac{1}{2}\text{C}_4\text{H}_4\text{O}_4.\frac{3}{4}\text{H}_2\text{O} \)

Batch Molecular Weight: 387.98

Physical Appearance: White solid

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

Storage: Store at RT

2. ANALYTICAL DATA

TLC: \( R_f = 0.65 \) (Dichloromethane:Methanol:Ammonia soln. [17:3:0.1])

Melting Point: Between 100 - 101°C

HPLC: Shows 98% purity

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

Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>61.91</td>
<td>61.95</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>8.7</td>
<td>8.68</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>3.61</td>
<td>3.6</td>
</tr>
</tbody>
</table>
Product Name: (±)-Bisoprolol hemifumarate
Catalog No.: 0914          Batch No.: 2

CAS Number: 104344-23-2
IUPAC Name: (±)-1-[4-[[2-(1-Methylethoxy)ethoxy]methyl]phenoxy]-3-[(1-methylethyl)amino]-2-propanol hemifumarate

Description:
A selective β₁-adrenergic antagonist. Has a Kᵦ of 2-3 nM at the β₁ receptor and a β₁/β₂ selectivity of approximately 100-fold.

Physical and Chemical Properties:
Batch Molecular Formula: C₁₈H₂₃NO₄·½C₄H₇O₄·¼H₂O
Batch Molecular Weight: 387.98
Physical Appearance: White solid
Minimum Purity: >98%

Storage: Store at RT
Solubility & Usage Info:
- water to 50 mM
- ethanol to 100 mM
- 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: