Product Name: Dobutamine hydrochloride
Catalog No.: 0515
Batch No.: 2

CAS Number: 49745-95-1
EC Number: 256-464-1
IUPAC Name: 4-[2-[[3-(4-Hydroxyphenyl)-1-methylpropyl]aminoethyl]1,2-benzenediol hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** \( \text{C}_{18}\text{H}_{23}\text{NO}_{3}\cdot\text{HCl} \)
- **Batch Molecular Weight:** 337.85
- **Physical Appearance:** White crystalline solid
- **Solubility:** DMSO to 100 mM
- **Storage:** Desiccate at RT

![Batch Molecular Structure]

2. ANALYTICAL DATA

- **TLC:** \( R_f = 0.45 \) (Chloroform:Methanol [10:1])
- **Melting Point:** Between 186 - 187°C
- **HPLC:** Shows 99.8% purity
- **\(^1\)H NMR:** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Microanalysis:**

<table>
<thead>
<tr>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>63.99</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>7.16</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>4.14</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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IUPAC Name: 4-[2-[[3-(4-Hydroxyphenyl)-1-methylpropyl]aminoethyl]1,2-benzenediol hydrochloride

Description:
β₁- and β₂-adrenoceptor agonist with some action at the α₁-adrenoceptor.

Physical and Chemical Properties:
Batch Molecular Formula: C₁₈H₂₃NO₅.HCl
Batch Molecular Weight: 337.85
Physical Appearance: White crystalline solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Desiccate 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:
Merck Index 12 3456.