Product Name: Nefazodone hydrochloride

Catalog No.: 2777          Batch No.: 1

CAS Number: 82752-99-6

IUPAC Name: 2-[[3-[4-[(3-Chlorophenyl)-1-piperazinyl]propyl]-5-ethyl-2,4-dihydro-4-(2-phenoxyethyl)-3H-1,2,4-triazol-3-one hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

   Batch Molecular Formula: C_{25}H_{32}ClN_{5}O_{2}.HCl
   Batch Molecular Weight: 506.47
   Physical Appearance: White crystalline solid
   Solubility: 1 eq. HCl to 10 mM
               DMSO to 25 mM
               ethanol to 10 mM
   Storage: Desiccate at RT

   Batch Molecular Structure:

2. ANALYTICAL DATA

   Melting Point: Between 186 - 188°C
   HPLC: Shows >99.9% 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>59.28</td>
<td>59.18</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>6.57</td>
<td>6.63</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>13.83</td>
<td>13.83</td>
</tr>
</tbody>
</table>

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

bio-techne.com  info@bio-techne.com  techsupport@bio-techne.com
North America  Tel: (800) 343 7475
China  info.cn@bio-techne.com  Tel: +86 (21) 52380373
Europe Middle East Africa  Tel: +44 (0)1235 529449
Rest of World  www.tocris.com/distributors  Tel: +1 612 379 2956
Product Name: Nefazodone hydrochloride  
CAS Number: 82752-99-6
IUPAC Name: 2-{3-[4-(3-Chlorophenyl)-1-piperazinyl]propyl}-5-ethyl-2,4-dihydro-4-(2-phenoxyethyl)-3H-1,2,4-triazol-3-one hydrochloride

Description:
Serotonin 5-HT$_{2A}$ receptor antagonist ($K_i$ = 5.8 nM) and inhibitor of serotonin and noradrenalin uptake ($IC_{50}$ values are 290 and 300 nM respectively). Displays no activity at 5-HT$_{1B}$ and 5-HT$_{1D}$ receptors. Active in models predictive of antidepressant potential.

Physical and Chemical Properties:
Batch Molecular Formula: C$_{25}$H$_{32}$ClN$_5$O$_2$.HCl
Batch Molecular Weight: 506.47
Physical Appearance: White crystalline solid
Minimum Purity: >99%

Batch Molecular Structure:

Storage: Desiccate at RT

Solubility & Usage Info:
1eq. HCl to 10 mM
DMSO to 25 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: