Product Name: (S)-Duloxetine hydrochloride
CAS Number: 136434-34-9
IUPAC Name: (+)-(S)-N-Methyl-3-(1-naphthyloxy)-3-(2-thienyl)propanamine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{18}\text{H}_{19}\text{NOS.HCl} \)
Batch Molecular Weight: 333.88
Physical Appearance: Off-white solid
Solubility:
- Water to 10 mM with gentle warming
- DMSO to 100 mM
Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.6% purity
\(^1\text{H NMR}:\) Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: \([\alpha]_D = +117.8\) (Concentration = 1, Solvent = Methanol)
Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>64.75</td>
<td>64.65</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>6.04</td>
<td>6.01</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>4.20</td>
<td>4.37</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
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
Tel:+1 612 379 2956

www.tocris.com/distributors
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Description:
High affinity, competitive 5-HT and noradrenaline (NA) re-uptake inhibitor ($K_i$ values are 8.5 and 45 nM for 5-HT and NA reuptake respectively in cortical synaptosomes; $IC_{50}$ values are 28 and 46 nM for 5-HT and NA reuptake respectively in rat hippocampal slices). Also blocks dopamine reuptake ($K_i = 300$ nM in striatal synaptosomes). Exhibits antidepressant and anxiolytic effects. Orally bioavailable.

Physical and Chemical Properties:
Batch Molecular Formula: $C_{18}H_{13}NOS.HCl$
Batch Molecular Weight: 333.88
Physical Appearance: Off-white solid

Minimum Purity: >99%

Storage: Store at RT

Solubility & Usage Info:
water to 10 mM with gentle warming
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: