Product Name: ICI 118,551 hydrochloride  
Catalog No.: 0821  
Batch No.: 5  

CAS Number: 72795-01-8  
IUPAC Name: (±)-erythro-(S*,S*)-1-[2,3-(Dihydro-7-methyl-1H-inden-4-yl)oxy]-3-[(1-methylethyl)amino]-2-butanol hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{17}H_{27}NO_{2}\cdot HCl  
Batch Molecular Weight: 313.87  
Physical Appearance: White solid  
Solubility: DMSO to 10 mM  
water to 10 mM  
Storage: Store at RT  

2. ANALYTICAL DATA

TLC: R_f = 0.68 (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])  
HPLC: Shows 100% purity  
^1H NMR: Consistent with structure  
Mass Spectrum: Consistent with structure  
Microanalysis: Carbon Hydrogen Nitrogen  
Theoretical 65.05 8.99 4.46  
Found 65.04 9.03 4.56

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

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Description:
Very selective β₂ adrenergic inverse agonist (Kᵢ values are 1.2, 120 and 257 nM for β₂, β₁, and β₃ receptors respectively). Active in vivo. Also available as part of the β-Adrenoceptor Antagonist Tocriset™.

Physical and Chemical Properties:
Batch Molecular Formula: C₁₁H₁₇NO₃.HCl
Batch Molecular Weight: 313.87
Physical Appearance: White solid
Minimum Purity: >98%

Storage: Store at RT

Solubility & Usage Info:
DMSO to 10 mM
water 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.

Licensing Information:
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References: