

Product Name: A 85380 dihydrochloride

Catalog No.: 5017

Batch No.: 2

CAS Number: 174740-86-4

IUPAC Name: 3-[(2S)-2-Azetidinylmethoxy]-pyridine dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₉H₁₂N₂O.2HCl.¼H₂O

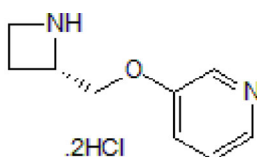
Batch Molecular Weight: 241.63

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows >99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -8.5 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	44.74	6.05	11.59
Found	44.82	6.04	11.5

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

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Description:

A 85380 dihydrochloride is a high affinity and selective $\alpha 4\beta 2$ nACh receptor agonist (K_i values are 0.05, 148 and 314 nM for $\alpha 4\beta 2$, $\alpha 7$ and $\alpha 1\beta 1\delta \gamma$ receptors respectively). Stimulates cation efflux in K177 cells expressing $\alpha 4\beta 2$.

Physical and Chemical Properties:

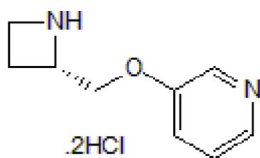
Batch Molecular Formula: $C_9H_{12}N_2O \cdot 2HCl \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 241.63

Physical Appearance: White solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Desiccate at RT. This product is packaged under an inert atmosphere.

Solubility & Usage Info:

water to 100 mM

DMSO to 100 mM

This product is supplied in lyophilized form. It may appear as a solid, gel or film and be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Abreo et al (1996) Novel 3-Pyridyl ethers with subnanomolar affinity for central neuronal nicotinic acetylcholine receptors. *J. Med. Chem.* **39** 817. PMID: 8632405.

Sullivan et al (1996) A-85380 [3-(2(S)-azetidylmethoxy) pyridine]; *in vitro* pharmacological properties of a novel, high affinity $\alpha 4\beta 2$ nicotinic acetylcholine receptor ligand. *Neuropharmacology* **35** 725. PMID: 8887981.

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