

Product Name: ABT 594 hydrochloride

Catalog No.: 6576

Batch No.: 1

CAS Number: 203564-54-9

IUPAC Name: (R)-5-(Azetidin-2-ylmethoxy)-2-chloropyridine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₉H₁₁ClN₂O.HCl.½H₂O

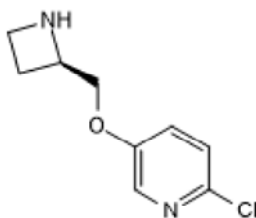
Batch Molecular Weight: 244.12

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



HCl

2. ANALYTICAL DATA

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +7.3 (Concentration = 0.52, Solvent = Methanol)

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 44.28 5.37 11.48

Found 44.21 5.25 11.21

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

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Description:

Selective $\alpha 4\beta 2$ nAChR agonist (EC_{50} = 140 nM for human $\alpha 4\beta 2$ nAChRs, in vitro). Exhibits >900-fold selectivity for $\alpha 4\beta 2$ nAChRs over other neurotransmitter receptors. Displays analgesic properties in various animal models of pain. Potentiates gabapentin mediated analgesia. Also demonstrates cognitive enhancement effects in rodent model of attention deficit.

Physical and Chemical Properties:

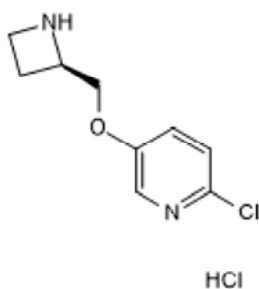
Batch Molecular Formula: $C_9H_{11}ClN_2O \cdot HCl \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 244.12

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM

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:

Mar et al (2017) MAM-E17 rat model impairments on a novel continuous performance task: effects of potential cognitive enhancing drugs. *Psychopharmacology (Berl)* **234** 2837. PMID: 28744563.

Munro et al (2010) Selective potentiation of gabapentin-mediated antinociception in the rat formalin test by the nicotinic acetylcholine receptor agonist ABT-594. *Neuropharmacology* **59** 208. PMID: 20562022.

Lynch et al (2005) ABT-594 (a nicotinic acetylcholine agonist): anti-allodynia in a rat chemotherapy-induced pain model. *Eur.J.Pharmacol.* **509** 43. PMID: 15713428.

Donnelly-Roberts et al (1998) ABT-594 [(R)-5-(2-azetidylmethoxy)-2-chloropyridine]: a novel, orally effective analgesic acting via neuronal nicotinic acetylcholine receptors: I. *In vitro* characterization. *J.Pharmacol.Exp.Ther.* **285** 777. PMID: 9580626.

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