

Product Name: NS 3861

Catalog No.: 4831

Batch No.: 2

CAS Number: 216853-60-0

IUPAC Name: 3-(3-Bromo-2-thienyl)-8-methyl-8-azabicyclo[3.2.1]oct-2-ene fumarate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₂H₁₄BrNS.C₄H₄O₄

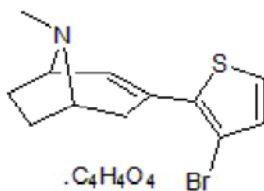
Batch Molecular Weight: 400.29

Physical Appearance: Off White solid

Solubility: water to 50 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows >99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	48.01	4.53	3.5
Found	48	4.5	3.52

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

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Description:

α 3 β 2 full agonist (EC_{50} = 1.6 μ M). Also α 3 β 4 partial agonist (EC_{50} = 1 μ M). Exhibits minimal activity at α 4 β 2 and α 4 β 4. Displays high affinity for α 3 β 4, α 4 β 4, α 3 β 2 and α 4 β 2 (K_i values are 0.62, 7.8, 25 and 55 nM respectively).

Physical and Chemical Properties:

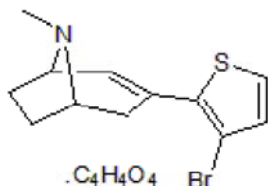
Batch Molecular Formula: C₁₂H₁₄BrNS.C₄H₄O₄

Batch Molecular Weight: 400.29

Physical Appearance: Off White solid

Minimum Purity: \geq 98%

Batch Molecular Structure:



References:

Harpsøe et al (2013) Molecular determinants of subtype-selective efficacies of cytisine and the novel compound NS3861 at heteromeric nicotinic acetylcholine receptors. *J.Biol.Chem.* **288** 2559. PMID: 23229547.

Storage: Desiccate at RT

Solubility & Usage Info:

water to 50 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.

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