

Product Name: Begacestat

Catalog No.: 4283

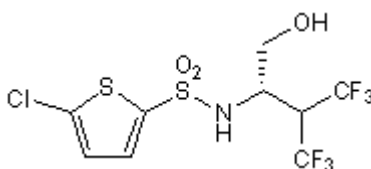
Batch No.: 1

CAS Number: 769169-27-9

IUPAC Name: 5-Chloro-N-[(1S)-3,3,3-trifluoro-1-(hydroxymethyl)-2-(trifluoromethyl)propyl]-2-thiophenesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₉H₈ClF₆NO₃S₂
Batch Molecular Weight: 391.74
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	27.59	2.06	3.58
Found	27.86	2.03	3.63

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

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Description:

γ-secretase inhibitor; selectively inhibits cleavage of amyloid precursor protein (APP) over Notch. Lowers levels of Aβ42 and Aβ40 (EC₅₀ values are 12.4 and 14.8 nM respectively in cells expressing human recombinant APP). Orally active.

Physical and Chemical Properties:

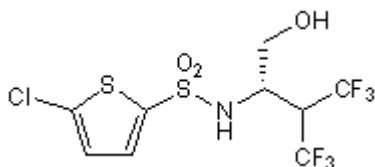
Batch Molecular Formula: C₉H₈ClF₆NO₃S₂

Batch Molecular Weight: 391.74

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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:

Mayer et al (2008) Discovery of begacestat, a Notch-1-sparing gamma secretase inhibitor for the treatment of Alzheimer's disease. *J.Med.Chem.* **51** 7348. PMID: 19012391.

Martone et al (2009) Begacestat (GSI-953): a novel, selective thiophene sulfonamide inhibitor of amyloid precursor protein γ-secretase for the treatment of Alzheimer's disease. *J.Pharmacol.Exp.Ther.* **331** 598. PMID: 19671883.

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