

Product Name: SID 26681509

Catalog No.: 3625

Batch No.: 2

CAS Number: 958772-66-2

IUPAC Name: *N*-[(1,1-Dimethylethoxy)carbonyl]-L-tryptophan-2-[[[2-[(2-ethylphenyl)amino]-2-oxoethyl]thio]carbonyl]hydrazide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₇H₃₃N₅O₅S·¼H₂O

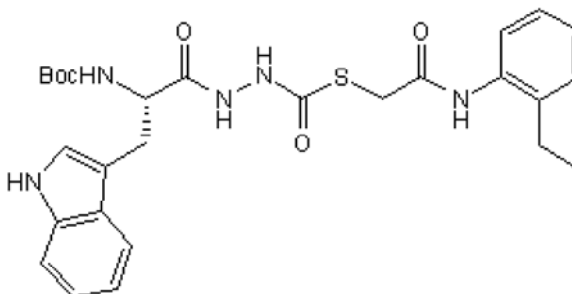
Batch Molecular Weight: 544.15

Physical Appearance: White solid

Solubility: DMSO to 50 mM
ethanol to 10 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -13.8 (Concentration = 0.5, Solvent = Acetic Acid)

Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	59.6	6.21	12.87
Found	59.25	5.99	12.72

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

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Description:

Potent and reversible human cathepsin L inhibitor (IC₅₀ = 56 nM). Displays no inhibitory activity at cathepsin G. Antimalarial; inhibits leishmaniasis.

Physical and Chemical Properties:

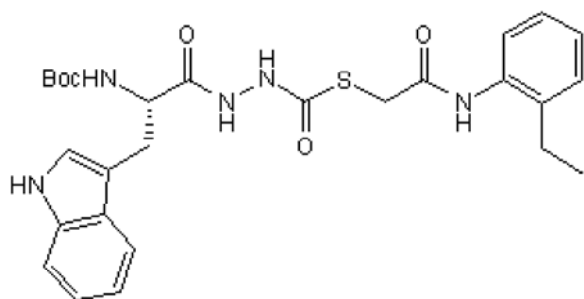
Batch Molecular Formula: C₂₇H₃₃N₅O₅S.¼H₂O

Batch Molecular Weight: 544.15

Physical Appearance: White solid

Minimum Purity: ≥97%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 mM

ethanol 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.

References:

Myers et al (2008) Identification and synthesis of a unique thiocarbazate cathepsin L inhibitor. *Bioorg.Med.Chem.Lett.* **18** 210. PMID: 18060772.

Shah et al (2008) Kinetic characterization and molecular docking of a novel, potent and selective slow-binding inhibitor of human cathepsin L. *Mol.Pharmacol.* **74** 34. PMID: 18403718.

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