

Product Name: NBD 556

Catalog No.: 5811

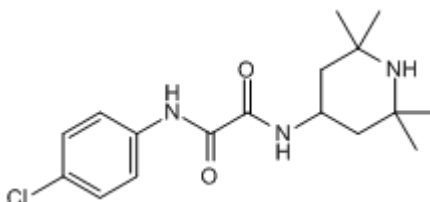
Batch No.: 1

CAS Number: 333353-44-9

IUPAC Name: *N*¹-(4-Chlorophenyl)-*N*²-(2,2,6,6-tetramethyl-4-piperidiny)ethanediamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₂₄ClN₃O₂
Batch Molecular Weight: 337.84
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 20 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.44	7.16	12.44
Found	60.45	7.11	12.23

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

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Description:

CD4 mimetic (IC₅₀ values are in low micromolar range, dependent on cell type and HIV strain). Recognizes and induces structural changes in HIV-1 envelope protein gp120, analogous to CD4 binding. Inhibits HIV-1 cell entry in CXCR4 and CCR5 expressing cell lines, by blocking virus-cell and cell-cell fusion.

Physical and Chemical Properties:

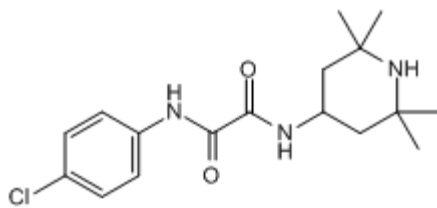
Batch Molecular Formula: C₁₇H₂₄ClN₃O₂

Batch Molecular Weight: 337.84

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Dogo-Isonagie et al (2012) Peptides from second extracellular loop of C-C chemokine receptor type 5 (CCR5) inhibit diverse strains of HIV-1. *J.Biol.Chem.* **287** 15076. PMID: 22403408.

Kwon et al (2012) Unliganded HIV-1 gp120 core structures assume the CD4-bound conformation with regulation by quaternary interactions and variable loops. *Proc.Natl.Acad.Sci.U.S.A.* **109** 5663. PMID: 22451932.

Zhao et al (2005) Identification of *N*-phenyl-*N*-(2,2,6,6-tetramethyl-piperidin-4-yl)-oxalamides as a new class of HIV-1 entry inhibitors that prevent gp120 binding to CD4. *Virology* **339** 213. PMID: 15996703.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 20 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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