

Product Name: A 286982

Catalog No.: 4228

Batch No.: 1

CAS Number: 280749-17-9

IUPAC Name: (2*E*)-1-(4-Acetyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-2-propen-1-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₇N₃O₄S·½H₂O

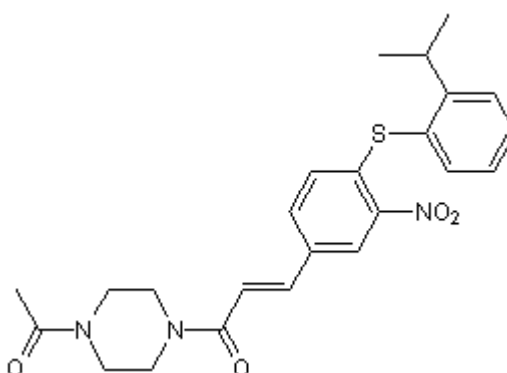
Batch Molecular Weight: 458.05

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.48 (Chloroform:Methanol [9:1])

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.93	6.05	9.17
Found	62.92	6.02	9.23

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Description:

Potent inhibitor of the LFA-1/ICAM-1 interaction (IC₅₀ values are 44 and 35 nM in LFA-1/ICAM-1 binding and LFA-1-mediated cell adhesion assays respectively).

Physical and Chemical Properties:

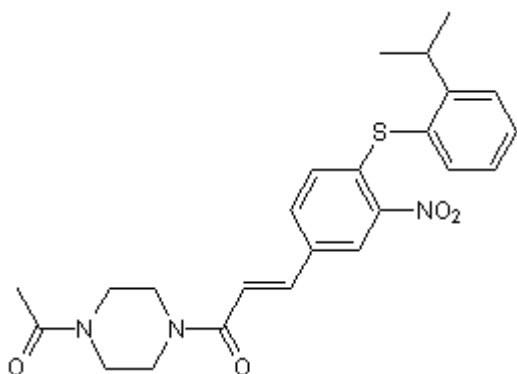
Batch Molecular Formula: C₂₄H₂₇N₃O₄S.¼H₂O

Batch Molecular Weight: 458.05

Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 50 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:

Liu *et al* (2000) Discovery of novel p-arylthio cinnamides as antagonists of leukocyte function-associated antigen-1/intracellular adhesion molecule-1 interaction. Identification of an additional binding pocket based on an anilino diaryl sulfide lead. *J.Med.Chem.* **43** 4025. PMID: 11052808.

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