

Product Name: A 205804

Catalog No.: 2524

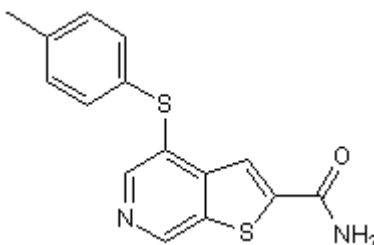
Batch No.: 1

CAS Number: 251992-66-2

IUPAC Name: 4-[(4-Methylphenyl)thio]thieno[2,3-c]pyridine-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₁₂N₂OS₂
Batch Molecular Weight: 300.39
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 10 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.46 (Dichloromethane:Methanol [9:1])
HPLC: Shows >98.9% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 59.98 | 4.03 | 9.32 |
| Found | 60.01 | 3.94 | 9.34 |

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

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IUPAC Name: 4-[(4-Methylphenyl)thio]thieno[2,3-c]pyridine-2-carboxamide

Description:

Selective inhibitor of E-selectin and ICAM-1 expression (IC₅₀ values are 20, 25 and > 1000 nM for TNF- α -induced E-selectin, ICAM-1 and VCAM-1 expression respectively). Effective inhibitor of cell-cell adhesion in an in vitro flow experiment.

Physical and Chemical Properties:

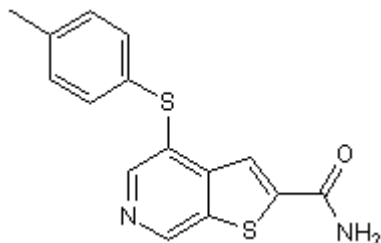
Batch Molecular Formula: C₁₅H₁₂N₂OS₂

Batch Molecular Weight: 300.39

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 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:

Stewart et al (2001) Discovery of inhibitors of cell adhesion molecule expression in human endothelial cells. 1. Selective inhibition of ICAM-1 and E-selectin expression. *J.Med.Chem.* **44** 988. PMID: 11300880.

Zhu et al (2001) Selective inhibition of ICAM-1 and E-selectin expression in human endothelial cells. 2. Aryl modifications of 4-(aryloxy)thieno[2,3-c]pyridines with fine-tuning at C-2 carbamides. *J.Med.Chem.* **44** 3469. PMID: 11585452.

Zhu et al (2002) Synthesis and mode of action of ¹²⁵I- and ³H-labeled thieno[2,3-c]pyridine antagonists of cell adhesion molecule expression. *J.Org.Chem.* **67** 943. PMID: 11856042.

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