

**Product Name:** A 205804

**Catalog No.:** 2524

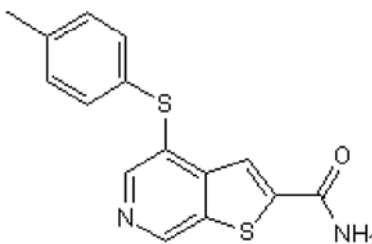
**Batch No.:** 1

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:** C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>OS<sub>2</sub>  
**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<sub>f</sub> = 0.46 (Dichloromethane:Methanol [9:1])  
**HPLC:** Shows 98.5% purity  
**<sup>1</sup>H 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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**Description:**

Selective inhibitor of E-selectin and ICAM-1 expression (IC<sub>50</sub> values are 20, 25 and > 1000 nM for TNF- $\alpha$ -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:**

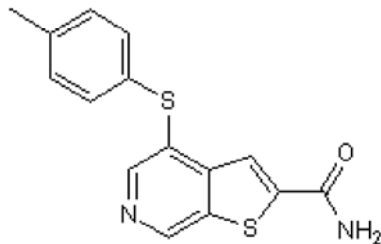
Batch Molecular Formula: C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>OS<sub>2</sub>

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:**

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

**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.

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