

Product Name: CBR 5884

Catalog No.: 5836

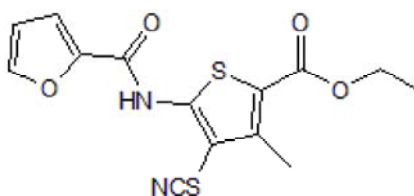
Batch No.: 1

CAS Number: 681159-27-3

IUPAC Name: Ethyl 5-[(2-furanylcarbonyl)amino]-3-methyl-4-thiocyanato-2-thiophenecarboxylate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₄H₁₂N₂O₄S₂
Batch Molecular Weight: 336.39
Physical Appearance: Yellow solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.2% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 49.99 | 3.6 | 8.33 |
| Found | 49.88 | 3.58 | 8.29 |

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

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IUPAC Name: Ethyl 5-[(2-furanylcarbonyl)amino]-3-methyl-4-thiocyanato-2-thiophenecarboxylate

Description:

Phosphoglycerate dehydrogenase (PHGDH) inhibitor (IC_{50} = 33 μ M). Decreases de novo serine synthesis in cancer cells. Inhibits proliferation of cancer cell lines having high PHGDH expression levels.

Physical and Chemical Properties:

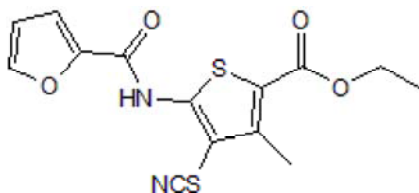
Batch Molecular Formula: $C_{14}H_{12}N_2O_4S_2$

Batch Molecular Weight: 336.39

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 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:

Mullarky *et al* (2016) Identification of a small molecule inhibitor of 3-phosphoglycerate dehydrogenase to target serine biosynthesis in cancers. *Proc.Natl.Acad.Sci.U.S.A.* **113** 1778. PMID: 26831078.

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