

Product Name: VU 0360223

Catalog No.: 4394

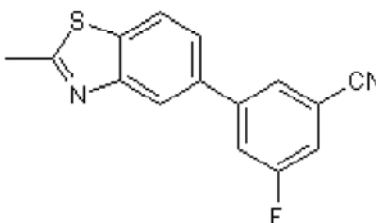
Batch No.: 1

CAS Number: 1274859-33-4

IUPAC Name: 3-Fluoro-5-(2-methyl-5-benzothiazolyl)-benzonitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₉FN₂S
Batch Molecular Weight: 268.31
Physical Appearance: Off-white solid
Solubility: DMSO to 25 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.34 (Ethyl acetate:Petroleum ether [1:4])
HPLC: Shows 99.3% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	67.15	3.38	10.44
Found	67.1	3.59	10.49

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

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Description:

Potent negative allosteric modulator of mGlu₅ (IC₅₀ = 61 nM).
Displays no activity at mGlu₁₋₄ and mGlu₇₋₈.

Physical and Chemical Properties:

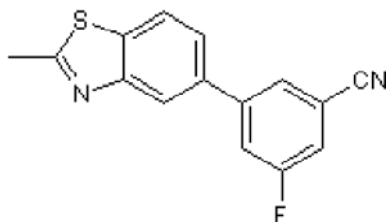
Batch Molecular Formula: C₁₅H₉FN₂S

Batch Molecular Weight: 268.31

Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 25 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:

Lindsley *et al* (2011) (3-cyano-5-fluorophenyl)biaryl negative allosteric modulators of mGlu₅: discovery of a new tool compound with activity in the OSS mouse model of addiction. *ACS Chem.Neurosci.* 2 471. PMID: 21927650.

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