

Product Name: A 967079

Catalog No.: 4716

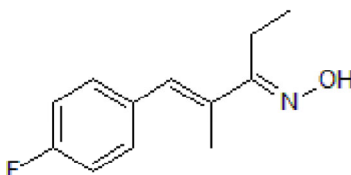
Batch No.: 5

CAS Number: 1170613-55-4

IUPAC Name: (1E,3E)-1-(4-Fluorophenyl)-2-methyl-1-pentene-3-one oxime

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₂H₁₄FNO.
Batch Molecular Weight: 207.24
Physical Appearance: Off White crystalline solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	69.55	6.81	6.76
Found	69.46	6.84	6.72

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

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Description:

A 967079 (also known as A-079) is a selective TRPA1 channel blocker (IC₅₀ values are 67 and 289 nM at human and rat TRPA1 receptors respectively) that displays 1000-fold selectivity for TRPA1 over other TRP channels, and is >150-fold selective over 75 other ion channels, enzymes and G-protein-coupled receptors. A 967079 exhibits analgesic effects in a rat osteoarthritic pain model.

Physical and Chemical Properties:

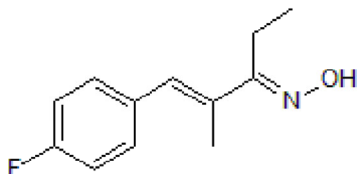
Batch Molecular Formula: C₁₂H₁₄FNO.

Batch Molecular Weight: 207.24

Physical Appearance: Off White crystalline solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Chen *et al* (2011) Selective blockade of TRPA1 channel attenuates pathological pain without altering noxious cold sensation or body temperature regulation. *Pain* **152** 1165. PMID: 21402443.

McGarughty *et al* (2010) TRPA1 modulation of spontaneous and mechanically evoked firing of spinal neurons in uninjured, osteoarthritic, and inflamed rats. *Mol.Pain* **6** 14. PMID: 20205719.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

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