

Product Name: VU 0238429

Catalog No.: 3634

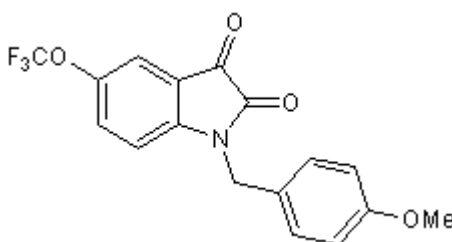
Batch No.: 1

CAS Number: 1160247-92-6

IUPAC Name: 1-(4-Methoxybenzyl)-5-trifluoromethoxyisatin

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₂F₃NO₄
Batch Molecular Weight: 351.28
Physical Appearance: orange solid
Solubility: DMSO to 100 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.9 (Ethyl acetate:Petroleum ether [1:1])
HPLC: Shows 98.9% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.13	3.44	3.99
Found	58.7	3.69	4.01

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

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Description:

Selective positive allosteric modulator of M₅ receptors (EC₅₀ values are 1.16, >30 and >30 μM at M₅, M₁ and M₃ receptors respectively). Displays no activity at M₂ and M₄ receptors.

Physical and Chemical Properties:

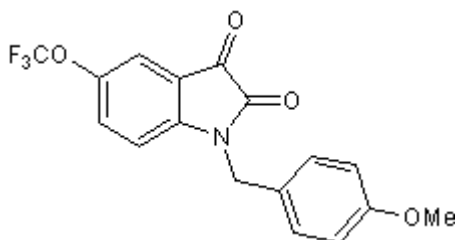
Batch Molecular Formula: C₁₇H₁₂F₃NO₄

Batch Molecular Weight: 351.28

Physical Appearance: orange solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

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:

Bridges et al (2009) Discovery of the first highly M₅-preferring muscarinic acetylcholine receptor ligand, an M₅ positive allosteric modulator derived from a series of 5-trifluoromethoxy *N*-benzyl isatins. *J.Med.Chem.* **52** 3445. PMID: 19438238.

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