

Product Name: UPF 648

Catalog No.: 4926

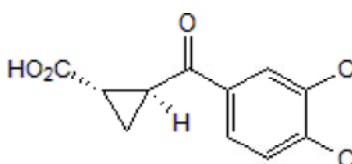
Batch No.: 2

CAS Number: 213400-34-1

IUPAC Name: (1S,2S)-2-(3,4-Dichlorobenzoyl)cyclopropanecarboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₁H₈Cl₂O₃
Batch Molecular Weight: 259.09
Physical Appearance: White solid
Solubility: ethanol to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Dichloromethane:Methanol [9:1])
HPLC: Shows 99.4% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = +163.3 (Concentration = 0.98, Solvent = Acetone)
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	50.99	3.11	
Found	51.14	3.05	

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

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IUPAC Name: (1S,2S)-2-(3,4-Dichlorobenzoyl)cyclopropanecarboxylic acid

Description:

Potent kynurenine 3-monooxygenase (kynurenine 3-hydroxylase; KMO) inhibitor (IC₅₀ = 20 nM). Increases kynurenic acid levels, and decreases 3-HK and QUIN levels in cerebrum and liver of neonatal rodents. Neuroprotective in a *Drosophila* model of Huntington's disease.

Physical and Chemical Properties:

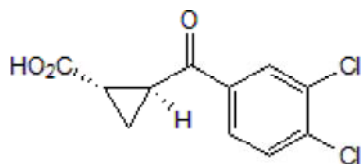
Batch Molecular Formula: C₁₁H₈Cl₂O₃

Batch Molecular Weight: 259.09

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

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. 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:

Amaral et al (2013) Structural basis of kynurenine 3-monooxygenase inhibition. *Nature* **496** 382. PMID: 23575632.

Campesan et al (2011) The kynurenine pathway modulates neurodegeneration in a *Drosophila* model of Huntington's disease. *Curr.Biol.* **21** 961. PMID: 21636279.

Amori et al (2009) On the relationship between the two branches of the kynurenine pathway in the rat brain *in vivo*. *J.Neurochem.* **109** 316. PMID: 19226371.

Ceresoli-Borroni et al (2007) Perinatal kynurenine 3-hydroxylase inhibition in rodents: pathophysiological implications. *J.Neurosci.Res.* **85** 845. PMID: 17279543.

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