

**Product Name:** INF 39

**Catalog No.:** 6341

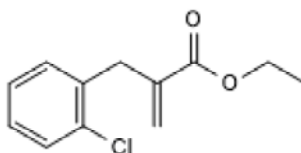
**Batch No.:** 1

CAS Number: 866028-26-4

IUPAC Name: Ethyl 2-(2-chlorobenzyl)acrylate

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>12</sub>H<sub>13</sub>ClO<sub>2</sub>·¼H<sub>2</sub>O  
**Batch Molecular Weight:** 229.18  
**Physical Appearance:** Colourless oil  
**Solubility:** Soluble in DMSO (supplied pre-dissolved in DMSO, 10mg/ml)  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.35 (9:1 petrol:EtOAc)  
**HPLC:** Shows 99.0% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	62.89	5.94	
Found	62.98	5.68	

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

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**Catalog No.:** 6341

**Batch No.:** 1

CAS Number: 866028-26-4

IUPAC Name: Ethyl 2-(2-chlorobenzyl)acrylate

**Description:**

Irreversible NLRP3 inhibitor (exhibits 52% inhibition of NLRP3 ATPase at 100  $\mu$ M). Inhibits IL-1 $\beta$  release, caspase activation and pyroptosis in THP-1 cells. Reduces inflammation in a rat colitis model. Exhibits low cytotoxicity.

**Physical and Chemical Properties:**

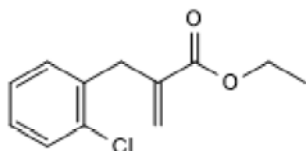
Batch Molecular Formula: C<sub>12</sub>H<sub>13</sub>ClO<sub>2</sub>·¼H<sub>2</sub>O

Batch Molecular Weight: 229.18

Physical Appearance: Colourless oil

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**CAUTION** - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

**Solubility & Usage Info:**

Soluble in DMSO (supplied pre-dissolved in DMSO, 10mg/ml)

This product is supplied dissolved in DMSO at a concentration of 10mg/mL

**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:**

**Cocco et al** (2017) Development of an acrylate derivative targeting the NLRP3 inflammasome for the treatment of inflammatory bowel disease. *J.Med.Chem.* **60** 3656. PMID: 28410442.

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