

**Product Name:** INF 4E

**Catalog No.:** 6172

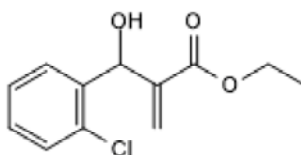
**Batch No.:** 1

CAS Number: 88039-46-7

IUPAC Name: Ethyl 2[(2-chlorophenyl)(hydroxy)methyl]acrylate

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>12</sub>H<sub>13</sub>ClO<sub>3</sub>  
**Batch Molecular Weight:** 240.68  
**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> = 0.2 (Ethyl acetate:Petroleum ether [9:1])  
**HPLC:** Shows 99% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	59.88	5.44	
Found	59.57	5.53	

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

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**Batch No.:** 1

CAS Number: 88039-46-7

IUPAC Name: Ethyl 2[(2-chlorophenyl)(hydroxy)methyl]acrylate

**Description:**

NLRP3 inflammasome and caspase-1 inhibitor ( $K_i = 9.6 \mu\text{M}$  for caspase-1). Inhibits Nigericin (Cat. No. 4312) or ATP (Cat.No. 3245) induced pyroptosis of PMA-differentiated and LPS-primed THP-1 cells and activates the Keap1-Nrf2 pathway.

**Physical and Chemical Properties:**

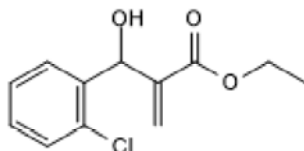
Batch Molecular Formula:  $\text{C}_{12}\text{H}_{13}\text{ClO}_3$

Batch Molecular Weight: 240.68

Physical Appearance: Colourless oil

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at  $-20^{\circ}\text{C}$

**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  $45\text{-}60^{\circ}\text{C}$  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  $-20^{\circ}\text{C}$  or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**References:**

Cocco *et al* (2014) Electrophilic warhead-based design of compounds preventing NLRP3 inflammasome-dependent pyroptosis. *J.Med.Chem.* **57** 10366. PMID: 25418070.

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