

## Certificate of Analysis

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**Product Name:** 4-Octyl itaconate

**Catalog No.:** 6662

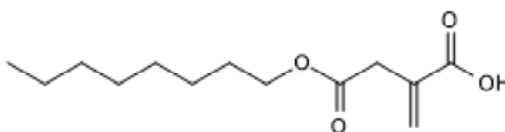
**Batch No.:** 2

CAS Number: 3133-16-2

IUPAC Name: 2-Methylenebutanedioic acid 4-octyl ester

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>13</sub>H<sub>22</sub>O<sub>4</sub>.  
**Batch Molecular Weight:** 242.31  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**HPLC:** Shows 100% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	64.44	9.15	
Found	64.58	9.28	

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

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**Catalog No.:** 6662

**Batch No.:** 2

CAS Number: 3133-16-2

IUPAC Name: 2-Methylenebutanedioic acid 4-octyl ester

**Description:**

4-Octyl itaconate activates Nrf2. Inhibits LPS-induced increases in IL-1 $\beta$  mRNA, HIF-1 $\alpha$  and IL-10 in macrophages. Decreases cytokine production in response to LPS in mice and prolongs survival. Cell permeable.

**Physical and Chemical Properties:**

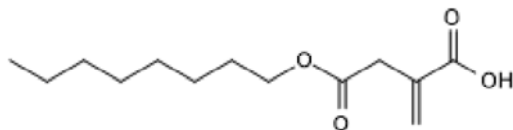
Batch Molecular Formula: C<sub>13</sub>H<sub>22</sub>O<sub>4</sub>.

Batch Molecular Weight: 242.31

Physical Appearance: White solid

**Minimum Purity:**  $\geq$ 98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**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:**

**Mills et al** (2018) Itaconate is an anti-inflammatory metabolite that activates Nrf2 via alkylation of KEAP1. *Nature* **556** 113. PMID: 29590092.

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