

Certificate of Analysis

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Product Name: 4-Octyl itaconate

Catalog No.: 6662

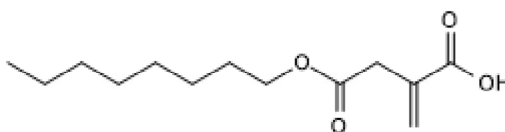
Batch No.: 2

CAS Number: 3133-16-2

IUPAC Name: 2-Methylenebutanedioic acid 4-octyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₃H₂₂O₄.
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 99.8% purity
¹H 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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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 β mRNA, HIF-1 α and IL-10 in macrophages. Decreases cytokine production in response to LPS in mice and prolongs survival. Cell permeable.

Physical and Chemical Properties:

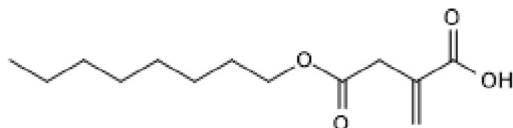
Batch Molecular Formula: C₁₃H₂₂O₄.

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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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