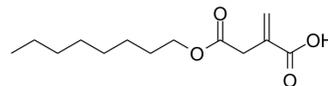


## 4-Octyl Itaconate

|                           |  |       |          |
|---------------------------|--|-------|----------|
| <b>Cat. No.:</b>          | HY-112675                                      |       |          |
| <b>CAS No.:</b>           | 3133-16-2                                      |       |          |
| <b>Molecular Formula:</b> | C <sub>13</sub> H <sub>22</sub> O <sub>4</sub> |       |          |
| <b>Molecular Weight:</b>  | 242.31   |       |          |
| <b>Target:</b>            | Keap1-Nrf2                                     |       |          |
| <b>Pathway:</b>           | NF-κB  |       |          |
| <b>Storage:</b>           | Powder   | -20°C | 3 years  |
|                           |  | 4°C   | 2 years  |
|                           | In solvent                                     | -80°C | 6 months |
|                           |  | -20°C | 1 month  |



### SOLVENT & SOLUBILITY

#### In Vitro

DMSO : 100 mg/mL (412.69 mM; Need ultrasonic)

| Preparing Stock Solutions | Solvent Concentration | Mass      |            |            |
|---------------------------|-----------------------|-----------|------------|------------|
|                           |                       | 1 mg      | 5 mg       | 10 mg      |
|                           | 1 mM                  | 4.1269 mL | 20.6347 mL | 41.2694 mL |
|                           | 5 mM                  | 0.8254 mL | 4.1269 mL  | 8.2539 mL  |
|                           | 10 mM                 | 0.4127 mL | 2.0635 mL  | 4.1269 mL  |

Please refer to the solubility information to select the appropriate solvent.

#### In Vivo

- Add each solvent one by one: 20% HP-β-CD in saline  
Solubility: 5 mg/mL (20.63 mM); Clear solution; Need ultrasonic and warming and heat to 60°C
- Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline  
Solubility: ≥ 2.5 mg/mL (10.32 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)  
Solubility: ≥ 2.5 mg/mL (10.32 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil  
Solubility: ≥ 2.5 mg/mL (10.32 mM); Clear solution
- Add each solvent one by one: 5% DMSO >> 40% PEG300 >> 5% Tween-80 >> 50% saline  
Solubility: ≥ 2.5 mg/mL (10.32 mM); Clear solution
- Add each solvent one by one: 5% DMSO >> 95% (20% SBE-β-CD in saline)  
Solubility: ≥ 2.5 mg/mL (10.32 mM); Clear solution

### BIOLOGICAL ACTIVITY

#### Description

4-Octyl Itaconate is a cell-permeable Itaconate derivative. Itaconate is an anti-inflammatory metabolite that activates Nrf2

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|                           |   |
|---------------------------|---|
|                           | via alkylation of KEAP1 <sup>[1]</sup> .  |
| IC <sub>50</sub> & Target | Nrf2 <sup>[1]</sup>   |
| In Vivo                   | 4-Octyl Itaconate (OI) is a cell-permeable itaconate derivative. 4-Octyl Itaconate is protective against lipopolysaccharide-induced lethality in vivo and decreases cytokine production <sup>[1]</sup> .<br>MCE has not independently confirmed the accuracy of these methods. They are for reference only. |

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## CUSTOMER VALIDATION

- Cell Metab. 2019 Aug.
- Mol Cell. 2022 May 25;S1097-2765(22)00443-9.
- Cell Death Dis. 2022 Feb 10;13(2):140.
- Free Radic Biol Med. 1 July 2022.
- Free Radic Biol Med. 2022 Feb 26;S0891-5849(22)00090-9.

See more customer validations on [www.MedChemExpress.com](http://www.MedChemExpress.com)

## REFERENCES

[1]. Mills EL, et al. Itaconate is an anti-inflammatory metabolite that activates Nrf2 via alkylation of KEAP1. Nature. 2018 Apr 5;556(7699):113-117.

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**Caution: Product has not been fully validated for medical applications. For research use only.**

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