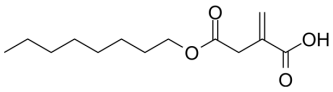
4-Octyl itaconate

Cat. No.:	HY-112675
CAS No.:	3133-16-2
Molecular Formula:	$C_{13}H_{22}O_4$
Molecular Weight:	242.31
Target:	Keap1-Nrf2
Pathway:	NF-κB
Storage:	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)
H_2O : < 0.1 mg/mL (ultrasonic;warming;heat to 80°C) (insoluble)

Preparing Stock Solutions

Mass / Solvent / Concentration	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

1. Add each solvent one by one: 20% HP-β-CD in saline
   Solubility: 10 mg/mL (41.27 mM); Suspended solution; Need ultrasonic
2. 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
3. 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
4. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (10.32 mM); Clear solution
5. 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
6. 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 via alkylation of KEAP1[1].
IC_{50} & Target	Nrf2[1]
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[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Cell Metab. 2019 Aug.
- Nat Commun. 2023 Sep 18;14(1):5778.
- Mol Cell. 2022 May 25;S1097-2765(22)00443-9.
- Int J Oral Sci. 2022 May 31;14(1):27.
- Proc Natl Acad Sci U S A. 2024 Apr 9;121(15):e2400675121.

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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.

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

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