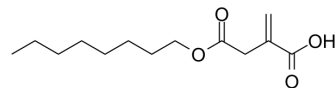


4-Octyl Itaconate

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)

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: 10 mg/mL (41.27 mM); Suspended solution; Need ultrasonic
- 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

	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.
- Oxid Med Cell Longev. 18 Aug 2021.
- FASEB J. 2019 Nov;33(11):12929-12940.
- Front Pharmacol. 25 May 2021.
- Ann Transl Med. 2021 Apr;9(8):712.

See more customer validations on 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.

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

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