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

2 years

In solvent -80°C 6 months

> -20°C 1 month

Product Data Sheet

SOLVENT & SOLUBILITY

In Vitro

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

H₂O: < 0.1 mg/mL (ultrasonic; warming; heat to 80°C) (insoluble)

Preparing Stock Solutions	Solvent Mass 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: 5 mg/mL (20.63 mM); Clear solution; Need ultrasonic and warming and heat to 60°C
- 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
- 7. Add each solvent one by one: PBS Solubility: 1 mg/mL (4.13 mM); Clear solution; Need ultrasonic and warming and heat to 60°C

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.
- J Nanobiotechnology. 2023 Oct 3;21(1):358.

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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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