Product Data Sheet

4-Octyl itaconate-¹³C₅-1

MedChemExpress

Cat. No.:	HY-112675S	
Molecular Formula:	C ₈ ¹³ C ₅ H ₂₂ O ₄	
Molecular Weight:	247.27	- 12
Target:	Isotope-Labeled Compounds	$\overbrace{{}_{{{}_{{{}_{{}_{{}_{{}_{{}_{{}_{{}_{$
Pathway:	Others	
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.	

BIOLOGICAL ACTIVITY		
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Description	4-Octyl itaconate- ¹³ C ₅ -1 is ¹³ C-labeled 4-Octyl itaconate (HY-112675). Itaconate is an anti-inflammatory metabolite that activates Nrf2 via alkylation of KEAP1.	
In Vitro	Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.	

REFERENCES

[1]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019 Feb;53(2):211-216.

[2]. 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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