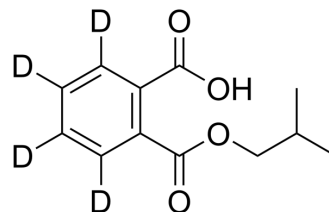


Monoisobutyl phthalic acid-d₄

Cat. No.:	HY-113220S		
CAS No.:	1219802-26-2		
Molecular Formula:	C ₁₂ H ₁₀ D ₄ O ₄		
Molecular Weight:	226.26		
Target:	Endogenous Metabolite		
Pathway:	Metabolic Enzyme/Protease		
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 (441.97 mM; Need ultrasonic)			
		Solvent Concentration	Mass	
			1 mg	5 mg
	Preparing Stock Solutions		10 mg	
	1 mM	4.4197 mL	22.0985 mL	44.1969 mL
	5 mM	0.8839 mL	4.4197 mL	8.8394 mL
	10 mM	0.4420 mL	2.2098 mL	4.4197 mL
Please refer to the solubility information to select the appropriate solvent.				
In Vivo	1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.5 mg/mL (11.05 mM); Clear solution			
	2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (11.05 mM); Clear solution			
	3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (11.05 mM); Clear solution			

BIOLOGICAL ACTIVITY

Description	Monoisobutyl phthalic acid-d ₄ is the deuterium labeled Monoisobutyl phthalic acid[1]. Monoisobutyl phthalic acid is a phthalate metabolite that is in human semen and in meconium[2].
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]. Kato K, et al. Quantifying phthalate metabolites in human meconium and semen using automated off-line solid-phase extraction coupled with on-line SPE and isotope-dilution high-performance liquid chromatography--tandem mass spectrometry. *Anal Chem*. 2006 Sep 15;78(18):6651-5.
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Caution: Product has not been fully validated for medical applications. For research use only.

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