# **Screening Libraries**

# **Product** Data Sheet

# Phthalic acid-d<sub>4</sub>

Cat. No.: HY-I0508S CAS No.: 87976-26-9 Molecular Formula:  $C_8H_2D_4O_4$ Molecular Weight: 170.16

Target: Isotope-Labeled Compounds

Pathway: Others

Powder Storage: -20°C 3 years

2 years

In solvent -80°C 6 months

> -20°C 1 month

### **SOLVENT & SOLUBILITY**

In Vitro

DMSO: 100 mg/mL (587.68 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	5.8768 mL	29.3841 mL	58.7682 mL
	5 mM	1.1754 mL	5.8768 mL	11.7536 mL
	10 mM	0.5877 mL	2.9384 mL	5.8768 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 (14.69 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (14.69 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (14.69 mM); Clear solution

## **BIOLOGICAL ACTIVITY**

Description

Phthalic acid-d<sub>4</sub> is the deuterium labeled Phthalic acid. Phthalic acid is the final common metabolite of phthalic acid esters (PAEs). Phthalic acid can be used for the synthesis of synthetic agents, such as isophthalic acid (IPA), and terephthalic acid (TPA). Phthalic acid has applications in the preparation of phthalate ester plasticizers[1].

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<sup>[1]</sup>.



## **REFERENCES**

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

[2]. Du Yeon Bang, et al. Toxicological Characterization of Phthalic Acid. Toxicol Res 2011;27:191–203

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

Tel: 609-228-6898 Fax: 609-228-5909

E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA

Page 2 of 2 www.MedChemExpress.com