Product Data Sheet

Benzyl benzoate-d₁₂

Cat. No.: HY-B0935S1

CAS No.: 352431-26-6Molecular Formula: $C_{14}D_{12}O_2$ Molecular Weight: 224.32

Target: Parasite; Endogenous Metabolite

Pathway: Anti-infection; Metabolic Enzyme/Protease

Storage: Pure form -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 (445.79 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg	
	1 mM	4.4579 mL	22.2896 mL	44.5792 mL	
	5 mM	0.8916 mL	4.4579 mL	8.9158 mL	
	10 mM	0.4458 mL	2.2290 mL	4.4579 mL	

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description Benzyl benzoate-d₁₂ is the deuterium labeled Benzyl benzoate[1]. Benzyl benzoate (Benzoic acid benzyl ester) is a fragrance

 $ingredient\ in\ cosmetic\ products.\ Benzyl\ benzoate\ can\ be\ used\ for\ the\ research\ of\ Scabies\ and\ Demodex-associated$

 $inflammatory\ skin\ conditions [2] [3] [4].$

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].

 $\label{eq:mce} \mbox{MCE has not independently confirmed the accuracy of these methods. They are for reference only.}$

REFERENCES

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

[2]. Johnson W, et, al. Safety Assessment of Benzyl Alcohol, Benzoic Acid and its Salts, and Benzyl Benzoate. Int J Toxicol. Nov/Dec 2017;36(3_suppl):5S-30S.

[3]. Jacob S, et, al. Treatment of Demodex-associated inflammatory skin conditions: A systematic review. Dermatol Ther. 2019 Nov32(6):e13103.								
[4]. Dressler C, et, al. The Treatment of Scabies. Dtsch Arztebl Int. 2016 Nov 14113(45):757-762.								
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