Benzyl benzoate

Cat. No.: HY-B0935

CAS No.: 120-51-4

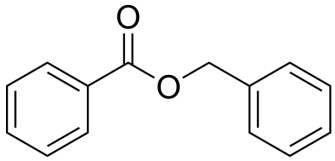
Molecular Formula: $C_{14}H_{12}O_2$

Molecular Weight: 212.24

Target: Parasite; Endogenous Metabolite; Angiotensin Receptor; Bacterial; Fungal

Pathway: Anti-infection; Metabolic Enzyme/Protease; GPCR/G Protein

Storage: 4°C, protect from light
* In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 50 mg/mL (235.58 mM)
* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	4.7116 mL	23.5582 mL	47.1165 mL
5 mM	0.9423 mL	4.7116 mL	9.4233 mL
10 mM	0.4712 mL	2.3558 mL	4.7116 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 (11.78 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (11.78 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (11.78 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Benzyl benzoate (Phenylmethyl benzoate) is an orally active anti-scabies agent, acaricide (EC_{50}= 0.06 g/m^2) and fungicide. Benzyl benzoate is an angiotensin II (Ang II) inhibitor with antihypertensive effects. Benzyl benzoate can be used in perfumes, pharmaceuticals and the food industry[1][2][3][4][5].

IC_{50} & Target

Mite

In Vitro

Benzyl benzoate (10000-50000 mg/L; 72 h) has toxic effects in allium root cells[3].
Benzyl benzoate (10-100 μM; 1-200 s) inhibits Ang II activity in a dose-dependent manner in 293T cells of human embryonic

kidney epithelium (mAT1a(HA)/293T) (IC_{50}=107 μg/mL) without cytotoxicity[5].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

Benzyl benzoate (25-100 mg/kg; p.o.; Once daily for 90 days) has no significant effects on body weight, relative organ weight, hematology, and biochemical outcomes in rats, but causes pathological changes in liver, kidney, thymus, prostate, and epididymal tissues in Sprague Dawley rats[4].

Benzyl benzoate (2-10 mg/kg; p.o.; Single dose) significantly inhibits Ang II (100 μg/kg) -induced hypertension in Std:ddY mice[5].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Hypertensive male Std:ddY mice model[5]
Dosage:	2 mg/kg, 10 mg/kg
Administration:	Oral gavage (p.o.); Single dose. Before Ang II treatment (100 μg/kg; Intraperitoneal injection (i.p.); Single dose)
Result:	Significantly inhibited the rise in systolic blood pressure induced by Ang II treatment.

Animal Model:	Sprague Dawley male rats model[4]
Dosage:	25 mg/kg, 100 mg/kg
Administration:	Oral gavage (p.o.); Once daily for 90 days
Result:	Induced hepatic portal vein blood supply, sinusoid sinus enlargement, monocyte infiltration, local lysis and cytoplasmic degeneration in rats. Induced renal tissue congestion, renal tubule degeneration, monocyte infiltration and histolysis in rats.Resulted in increased number of Hassall's bodies, elevated lipids, degeneration, congestion, fibrosis and lymphocytopenia in the thymus of rats. Resulted in vacuolation and irregular secretion of the prostate in male reproductive system tissue, increased connective tissue of the epididymis and presence of cells in the lumen. In the male reproductive system tissues, resulted in vacuolation and irregular secretion in the prostate, increased connective tissue of the epididymis, and presence of cells in the lumen.

CUSTOMER VALIDATION

- Int J Polym Anal Ch. 2021 Jan 7.

See more customer validations on www.MedChemExpress.com

REFERENCES

[1]. Bachewar NP, et al. Comparison of safety, efficacy, and cost effectiveness of benzyl benzoate, permethrin, and ivermectin in patients of scabies. Indian J Pharmacol. 2009 Feb;41(1):9-14.

[2]. Raynaud S, et al. Squamocin and benzyl benzoate, acaricidal components of Uvaria pauci-ovulata bark extracts. Planta Med. 2000 Mar;66(2):173-5.

[3]. Acar A, et al. Investigation of benzyl benzoate toxicity with anatomical, physiological, cytogenetic and biochemical parameters in in vivo[J]. Caryologia, 2020, 73(3).

[4]. Kılıç Süloğlu A, et al. Toxicity of benzyl benzoate as a food additive and pharmaceutical agent. Toxicol Ind Health. 2022 Apr;38(4):221-233.

[5]. Ohno O, et al. Inhibitory effects of benzyl benzoate and its derivatives on angiotensin II-induced hypertension. Bioorg Med Chem. 2008 Aug 15;16(16):7843-52.

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