(±)-2-Propyl-4-pentenoic acid

Cat. No.: HY-124087

CAS No.: 1575-72-0

Molecular Formula: $C_8H_{14}O_2$

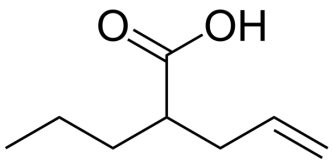
Molecular Weight: 142.2

Target: Drug Metabolite

Pathway: 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 (703.23 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	7.0323 mL	35.1617 mL	70.3235 mL
5 mM	1.4065 mL	7.0323 mL	14.0647 mL
10 mM	0.7032 mL	3.5162 mL	7.0323 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 (17.58 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (17.58 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (17.58 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

(±)-2-Propyl-4-pentenoic acid (4-en-VPA) is a major toxic metabolite of Valproic acid. (±)-2-Propyl-4-pentenoic acid exhibits neuroteratogenicity[1][2].

In Vitro

(±)-2-Propyl-4-pentenoic acid (1 mM; 26 h) induces approximately 50% of dysmorphogenic mouse embryos[2].

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

REFERENCES

[1]. W Tang, et, al. A comparative investigation of 2-propyl-4-pentenoic acid (4-ene VPA) and its alpha-fluorinated analogue: phase II metabolism and pharmacokinetics. Drug Metab Dispos. 1997 Feb;25(2):219-27.

[2]. Gofflot F, et, al. In vitro neuroteratogenicity of valproic acid and 4-en-VPA. Neurotoxicol Teratol. Jul-Aug 1995;17(4):425-35.

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