

Isobutylshikonin

Chemical Properties

CAS No. : 52438-12-7

Formula: C₂₀H₂₂O₆

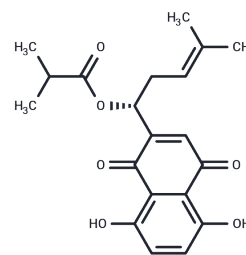
Molecular Weight: 358.39

Storage:

Keep away from direct sunlight, Keep away from moisture

Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Actual storage temperature shall be subject to the COA.



Biological Description

Description	Isobutylshikonin exhibits obvious antioxidant activities, it exerts very good radical scavenging activities toward ABTS ⁺ but shows moderate inhibition of DPPH [•] .
Targets(IC ₅₀)	Others
In vitro	Five red shikonin pigments, deoxyshikonin, shikonin, acetylshikonin, Isobutylshikonin, and beta-hydroxyisovalerylshikonin, were isolated from the roots of <i>Lithospermum erythrorhizon</i> cultivated in Korea. The purified pigments were red, purple, and blue at acidic, neutral, and alkaline pH values, respectively. Physical stability of the purified pigments against heat and light in an aqueous solution was examined for possible value-added food colorants. The thermal degradation reactions were carried out at pH 3.0 (50 mM glycine buffer) in 50% EtOH/H ₂ O. Deoxyshikonin (t _{1/2} = 14.6 h, 60 degrees C) and isobutylshikonin (t _{1/2} = 19.3 h, 60 degrees C) are relatively less stable than other shikonin derivatives (t _{1/2} = 40-50 h, 60 degrees C). Activation energies of thermal degradation of the isolated pigments were calculated. The activation energy of deoxyshikonin was the highest (12.5 kcal mol ⁻¹) and that of beta-hydroxyisovalerylshikonin was the lowest (1.71 kcal mol ⁻¹) value[1]

Solubility Information

Solubility	DMSO: 14.55 mg/mL (40.6 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Saline: 1.45 mg/mL (4.05 mM), Solution. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.7903 mL	13.9513 mL	27.9026 mL
5 mM	0.5581 mL	2.7903 mL	5.5805 mL
10 mM	0.279 mL	1.3951 mL	2.7903 mL
50 mM	0.0558 mL	0.279 mL	0.5581 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Cho MH, Paik YS, Hahn TR. Physical stability of shikonin derivatives from the roots of *Lithospermum erythrorhizon* cultivated in Korea. *J Agric Food Chem*. 1999 Oct;47(10):4117-20.

H Damianakos, et al. Shikonin pigments from hairy root culture of *Lithospermum canescens*. *Planta Med* 2007; 73 - P_185.

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