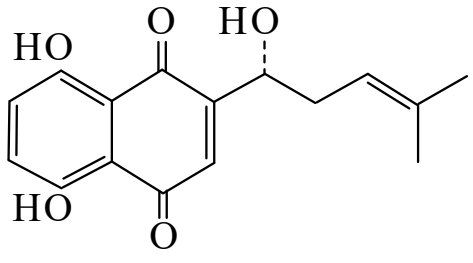
>>**Entry Name: 5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl)-1,4-naphthalenedione,** 9CI
ENTRY UNDER REVIEW
Synonym(s): Shikonin. Alkannin. Arnebin IV. Anchusaic acid. Anchusin. Alkanna red. Alkhanin. Shikalkin



(*R*)-*form*

Related CAS Registry Numbers(s): 38222-13-8 85921-41-1

Molecular Formula: $C_{16}H_{16}O_5$
Molecular Weight: 288.299
Accurate Mass: 288.099775
Percentage Composition: C 66.66%; H 5.59%; O 27.75%
General Statement: Historically Shikonin was the (*R*)-form and Alkannin (=Anchusin etc.) the (*S*)-form. Shikalkin was the (±)-form

>>**Variant:** (*R*)-form

CAS Registry Number: 517-89-5

Molecular Formula: $C_{16}H_{16}O_5$
Molecular Weight: 288.299
Accurate Mass: 288.099775
Percentage Composition: C 66.66%; H 5.59%; O 27.75%
Biological Source: Isol. from *Lithospermum erythrorhizon, Lithospermum officinale, Lithospermum euchromum, Arnebia nobilis* and *Arnebia tibetana*
Biological Use/Importance: Antibacterial agent
Physical Description: Red-brown cryst. (C_6H_6)
Melting Point: Mp 148° (143°)
Optical Rotation: $[\alpha]_{Hg}^{20}$ +135 (C_6H_6)
Calculated Log P Data: Log P 1.84 (calc)
UV: [base] λ_{max} (solvent not reported) (Derep) [neutral] λ_{max} 276 (ε 20000); 488 (ε 1200); 525 (ε 8700); 563 (ε 5900) (MeOH) (Derep)
Other Data: Component of Tokyo violet
Hazard & Toxicity: LD_{50} (mus, orl) >1000 mg/kg; LD_{50} (mus, ipr) 20 mg/kg

>>**Derivative:** $O^{1'}$-Ac
Synonym(s): Shikonin acetate. Acetylshikonin

CAS Registry Number: 24502-78-1

Molecular Formula: $C_{18}H_{18}O_6$
Molecular Weight: 330.337
Accurate Mass: 330.11034
Percentage Composition: C 65.45%; H 5.49%; O 29.06%
Biological Source: Isol. from *Lithospermum erythrorhizon, Lithospermum euchromum* and *Jatropha glandulifera*
Physical Description: Red prisms or reddish-violet needles
Melting Point: Mp 85-86°. Mp 106-107°

>>**Derivative:** $O^{1'}$-(Methoxyacetyl)
Synonym(s): Methoxyacetylshikonin

CAS Registry Number: 106265-27-4

Molecular Formula: $C_{19}H_{20}O_7$
Molecular Weight: 360.363
Accurate Mass: 360.120905
Percentage Composition: C 63.33%; H 5.59%; O 31.08%
Biological Source: Constit. of *Arnebia euchroma*