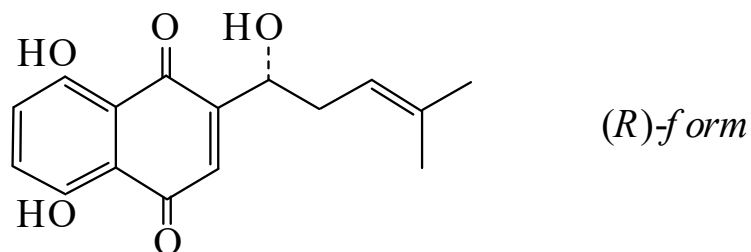




>>Entry Name: 5,8-Dihydroxy-2-(1-hydroxy-4-methyl-3-pentenyl)-1,4-naphthalenedione, 9CI

ENTRY UNDER REVIEW

Synonym(s): Shikonin. Alkannin. Arnebin IV. Anchusaic acid. Anchusin. Alkanna red. Alkhanin. Shikalkin



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

Molecular Formula: C<sub>16</sub>H<sub>16</sub>O<sub>5</sub>

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<sub>16</sub>H<sub>16</sub>O<sub>5</sub>

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<sub>6</sub>H<sub>6</sub>)

Melting Point: Mp 148° (143°)

Optical Rotation: [α]<sub>D</sub><sup>20</sup> +135 (C<sub>6</sub>H<sub>6</sub>)

Calculated Log P Data: Log P 1.84 (calc)

UV: [base] λ<sub>max</sub> (solvent not reported) (Derep) [neutral] λ<sub>max</sub> 276 (ε 20000); 488 (ε 1200); 525 (ε 8700); 563 (ε 5900) (MeOH) (Derep)

Other Data: Component of Tokyo violet

Hazard & Toxicity: LD<sub>50</sub> (mus, orl) >1000 mg/kg; LD<sub>50</sub> (mus, ipr) 20 mg/kg

>>Derivative: O<sup>I</sup>-Ac

Synonym(s): Shikonin acetate. Acetylshikonin

CAS Registry Number: 24502-78-1

Molecular Formula: C<sub>18</sub>H<sub>18</sub>O<sub>6</sub>

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<sup>I</sup>-(Methoxyacetyl)

Synonym(s): Methoxyacetylshikonin

CAS Registry Number: 106265-27-4

Molecular Formula: C<sub>19</sub>H<sub>20</sub>O<sub>7</sub>

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*