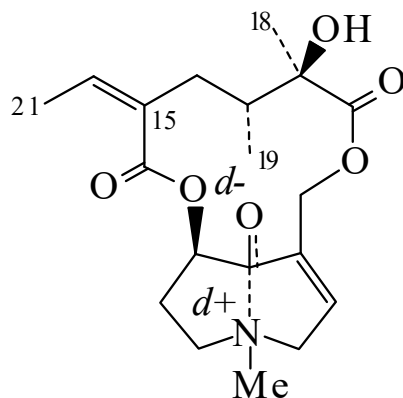




>>Entry Name: Senkirkine

Synonym(s): 12-Hydroxy-4-methyl-4,8-secosenecionan-8,11,16-trione, 9Cl. Renardine



CAS Registry Number: 2318-18-5

Related CAS Registry Numbers(s): 6882-01-5

Molecular Formula: C<sub>19</sub>H<sub>27</sub>NO<sub>6</sub>

Molecular Weight: 365.425

Accurate Mass: 365.183839

Percentage Composition: C 62.45%; H 7.45%; N 3.83%; O 26.27%

Biological Source: Alkaloid from *Senecio* spp., *Nardosmia laevigata*, *Farfugium japonicum*, *Crotalaria laburnifolia* etc. (Compositae, Leguminosae)

Physical Description: Bevelled plates (EtOAc or Me<sub>2</sub>CO)

Melting Point: Mp 196.5-197.5°

Optical Rotation:  $[\alpha]_D^{25} -16$  (c, 1.89 in MeOH)

Solubility: BERDY SOL: Sol. MeOH, CHCl<sub>3</sub>; poorly sol. H<sub>2</sub>O

pKa Value: pK<sub>a</sub> 6.4

UV: [neutral]  $\lambda_{max}$  219 ( $\epsilon$  10500) (MeOH) (Berdy)

Hazard & Toxicity: LD<sub>50</sub> (rat, ipr) 220 mg/kg. Exp. neoplastic agent, hepatotoxic

>>Derivative: Picrate

Physical Description: Yellow rods (EtOH aq.)

Melting Point: Mp 225-225.5° (219-220°)

>>Derivative: Ac

Synonym(s): *O*-Acetylsenkirkine

CAS Registry Number: 53092-44-7

Molecular Formula: C<sub>21</sub>H<sub>29</sub>NO<sub>7</sub>

Molecular Weight: 407.463

Accurate Mass: 407.194404

Percentage Composition: C 61.90%; H 7.17%; N 3.44%; O 27.49%

Biological Source: Alkaloid from *Senecio kirkii* (Compositae)

Physical Description: Needles (EtOAc/Me<sub>2</sub>CO)

Melting Point: Mp 195-196°

Optical Rotation:  $[\alpha]_D^{25} -34$  (c, 0.44 in MeOH)

>>Derivative: 1*R*,2-Dihydro

Synonym(s): Dihydrosenkirkine

CAS Registry Number: 135574-55-9

Molecular Formula: C<sub>19</sub>H<sub>29</sub>NO<sub>6</sub>

Molecular Weight: 367.441

Accurate Mass: 367.199489

Percentage Composition: C 62.11%; H 7.95%; N 3.81%; O 26.13%

Biological Source: Alkaloid from *Senecio integrifolius* var. *fauriri* (Asteraceae)

Other Data: Exists in equilib. as two ring structs.