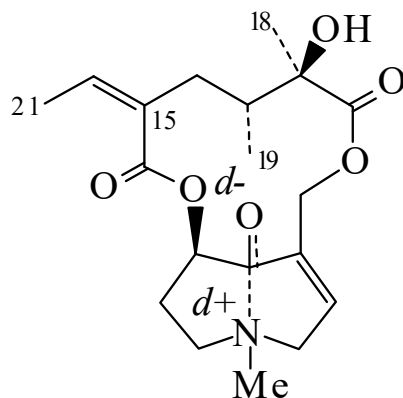




>>Entry Name: Senkirkine

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



CAS Registry Number: 2318-18-5

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

Molecular Formula: $C_{19}H_{27}NO_6$

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_2CO)

Melting Point: Mp 196.5-197.5°

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

Solubility: BERDY SOL: Sol. MeOH, $CHCl_3$; poorly sol. H_2O

pKa Value: pK_a 6.4

UV: [neutral] λ_{max} 219 (ϵ 10500) (MeOH) (Berdy)

Hazard & Toxicity: LD_{50} (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: $C_{21}H_{29}NO_7$

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_2CO)

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: $C_{19}H_{29}NO_6$

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.