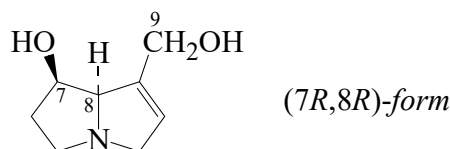




>>Entry Name: 2,3,5,7a-Tetrahydro-1-hydroxy-1*H*-pyrrolizine-7-methanol, 9Cl

Synonym(s): 7-Hydroxy-1-hydroxymethyl-1,2-didehydropyrrolizidine



Related CAS Registry Numbers(s): 875-22-9 6029-83-0 17690-54-9 133738-52-0 133738-53-1

Molecular Formula: C₈H₁₃NO₂

Molecular Weight: 155.196

Accurate Mass: 155.094629

Percentage Composition: C 61.91%; H 8.44%; N 9.03%; O 20.62%

>>Variant: (7*R*,8*R*)-form

Synonym(s): Retronecine

CAS Registry Number: 480-85-3

Molecular Formula: C₈H₁₃NO₂

Molecular Weight: 155.196

Accurate Mass: 155.094629

Percentage Composition: C 61.91%; H 8.44%; N 9.03%; O 20.62%

Physical Description: Cryst. (Me₂CO or by subl.)

Melting Point: Mp 121-122°

Optical Rotation: [α]_D²⁶ +50.2 (EtOH)

Solubility: Sol. H₂O, EtOH; spar. sol. Et₂O; BERDY SOL: Sol. EtOH, H₂O; fairly sol. Me₂CO, CHCl₃; poorly sol. Et₂O, hexane

pKa Value: p*K*_a 8.88 (26°)

UV: [neutral] λ_{max} 0 (end) (ε) (MeOH) (Derep)

Other Data: Does not form a picrate

Hazard & Toxicity: LD₅₀ (mus, ivn) 634 mg/kg ; BERDY HAZD : LD₅₀ (mus, ivn) 634 mg/kg

>>Derivative: Hydrochloride

Melting Point: Mp 162-163°

Optical Rotation: [α]_D¹⁵ -16 (EtOH)

>>Derivative: *N*-Oxide

Synonym(s): Retronecine *N*-oxide

CAS Registry Number: 6870-33-3

Molecular Formula: C₈H₁₃NO₃

Molecular Weight: 171.196

Accurate Mass: 171.089544

Percentage Composition: C 56.13%; H 7.65%; N 8.18%; O 28.04%

Biological Source: Alkaloid from *Senecio caudatus* and *Werneria decora*

>>Derivative: *O*⁷-(3-Methylbutanoyl)

Synonym(s): *O*⁷-(3-Methylbutanoyl)retronecine

CAS Registry Number: 63503-35-5

Molecular Formula: C₁₃H₂₁NO₃

Molecular Weight: 239.314

Accurate Mass: 239.152144

Percentage Composition: C 65.25%; H 8.84%; N 5.85%; O 20.06%

Biological Source: Constit. of *Crotalaria scassellatii*