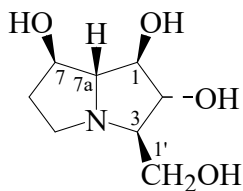




>>Entry Name: 1,2,7-Trihydroxy-3-(hydroxymethyl)-1*H*-pyrrolizidine

Synonym(s): Hexahydro-1,2,7-trihydroxy-1*H*-pyrrolizine-3-methanol



(1*R*,2*R*,3*R*,7*R*,7*aR*)-form

Molecular Formula: C₈H₁₅NO₄

Molecular Weight: 189.211

Accurate Mass: 189.100109

Percentage Composition: C 50.78%; H 7.99%; N 7.40%; O 33.82%

>>Variant: (1*R*,2*R*,3*R*,7*R*,7*aR*)(?)-form

Synonym(s): 7,8-Diepialexine. 7,7*a*-Diepialexine. 7-Epiaustraline

CAS Registry Number: 126655-21-8

Extra CAS Registry Numbers(s): 126655-01-4

Molecular Formula: C₈H₁₅NO₄

Molecular Weight: 189.211

Accurate Mass: 189.100109

Percentage Composition: C 50.78%; H 7.99%; N 7.40%; O 33.82%

Use/Importance: Weak inhibitor of glucosidase activity

Physical Description: Oil (natural), cryst. (synthetic)

Melting Point: Mp 193-194° (synthetic)

Optical Rotation: $[\alpha]_{\text{D}}^{20} +11.6$ (c, 0.37 in H₂O) (nat.). $[\alpha]_{\text{D}}^{23} -13$ (c, 0.55 in H₂O) (synthetic)

Calculated Log P Data: Log P -2.17 (calc)

Other Data: The assigned struct. of the nat. alkaloid is incorrect as it was not identical with the synthetic material. No alternative struct. has been proposed (1998)

>>Variant: (1*R*,2*R*,3*R*,7*R*,7*aS*)-form

CAS Registry Number: 121588-45-2

Molecular Formula: C₈H₁₅NO₄

Molecular Weight: 189.211

Accurate Mass: 189.100109

Percentage Composition: C 50.78%; H 7.99%; N 7.40%; O 33.82%

Source/Synthesis: Synthetic

Physical Description: Syrup

Optical Rotation: $[\alpha]_{\text{D}}^{20} -10.6$ (c, 0.56 in H₂O)

>>Variant: (1*R*,2*R*,3*R*,7*S*,7*aR*)-form

Synonym(s): Australine. 8-Epialexine. 7*a*-Epialexine

CAS Registry Number: 118396-02-4

Molecular Formula: C₈H₁₅NO₄

Molecular Weight: 189.211

Accurate Mass: 189.100109

Percentage Composition: C 50.78%; H 7.99%; N 7.40%; O 33.82%

Use/Importance: Potent and specific inhibitor of amyloglucosidase

Physical Description: Prisms (Me₂CO)

Melting Point: Mp 148-149°

Optical Rotation: $[\alpha]_{\text{D}}^{26} +19.3$ (c, 2.09 in MeOH)

Solubility: BERDY SOL: Sol. H₂O, MeOH

UV: [neutral] λ_{max} (H₂O) (Berdy)