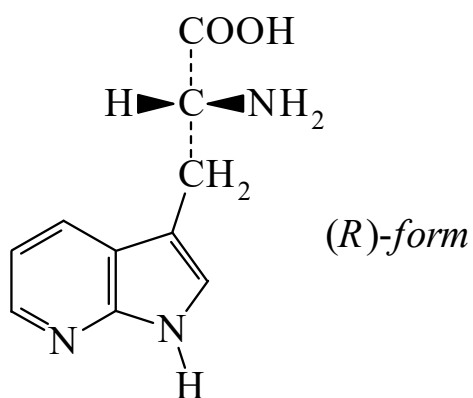




>>Entry Name: 2-Amino-3-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)propanoic acid

Synonym(s): α -Amino-1*H*-pyrrolo[2,3-*b*]pyridine-3-propanoic acid, 9Cl. 1*H*-Pyrrolo[2,3-*b*]pyridine-3-alanine. 7-Azatryptophan



CAS Registry Number: 1137-00-4

Molecular Formula: C₁₀H₁₁N₃O₂

Molecular Weight: 205.216

Accurate Mass: 205.085127

Percentage Composition: C 58.53%; H 5.40%; N 20.48%; O 15.59%

Use/Importance: Alternative to tryptophan as optical probe of protein struct. and dynamics

>>Variant: (*R*)-form

CAS Registry Number: 134235-82-8

Molecular Formula: C₁₀H₁₁N₃O₂

Molecular Weight: 205.216

Accurate Mass: 205.085127

Percentage Composition: C 58.53%; H 5.40%; N 20.48%; O 15.59%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 260-261 dec.°

Optical Rotation: $[\alpha]_{\text{D}}^{22} -1.2$ (c, 0.5 in H₂O)

>>Variant: (*S*)-form

CAS Registry Number: 49758-35-2

Molecular Formula: C₁₀H₁₁N₃O₂

Molecular Weight: 205.216

Accurate Mass: 205.085127

Percentage Composition: C 58.53%; H 5.40%; N 20.48%; O 15.59%

Optical Rotation: $[\alpha]_{\text{D}}^{25} +14.7$ (c, 0.3 in 1*M* HCl)

>>Variant: ($\pm$)-form

CAS Registry Number: 7303-50-6

Molecular Formula: C₁₀H₁₁N₃O₂

Molecular Weight: 205.216

Accurate Mass: 205.085127

Percentage Composition: C 58.53%; H 5.40%; N 20.48%; O 15.59%

Physical Description: Needles + 1H₂O (H₂O)

Melting Point: Mp 257-259 dec.° (monohydrate)

Sigma: A1632

>>Derivative: *N* ^{α} -Ac

CAS Registry Number: 63024-18-0

Molecular Formula: C₁₂H₁₃N₃O₃

Molecular Weight: 247.253

Accurate Mass: 247.095692

Percentage Composition: C 58.29%; H 5.30%; N 16.99%; O 19.41%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 240-243°

References:

Robison, M.M. *et al.*, *J.A.C.S.*, 1955, **77**, 457, (*synth*)

Sloan, M.J. *et al.*, *Bioorg. Med. Chem. Lett.*, 1992, **2**, 1053, (*S*-form, *synth*, *ir*, *pmr*)

Sánchez-Obregón, R. *et al.*, *Can. J. Chem.*, 1992, **70**, 1531, (*R*-form, *synth*, *ir*, *pmr*)

Lecointe, L. *et al.*, *Tetrahedron: Asymmetry*, 1998, **9**, 1753-1758, (*R*-form, *S*-form, *synth*, *pmr*, *hplc*)