



>>Entry Name: *N*-Glycylisoleucine



Molecular Formula: C₈H₁₆N₂O₃

Molecular Weight: 188.226

Accurate Mass: 188.116093

Percentage Composition: C 51.05%; H 8.57%; N 14.88%; O 25.50%

>>Variant: D-form

Molecular Formula: C₈H₁₆N₂O₃

Molecular Weight: 188.226

Accurate Mass: 188.116093

Percentage Composition: C 51.05%; H 8.57%; N 14.88%; O 25.50%

Optical Rotation: $[\alpha]_{\text{D}}^{25} +14$ (c, 2 in H₂O)

>>Variant: L-form

CAS Registry Number: 19461-38-2

Molecular Formula: C₈H₁₆N₂O₃

Molecular Weight: 188.226

Accurate Mass: 188.116093

Percentage Composition: C 51.05%; H 8.57%; N 14.88%; O 25.50%

Optical Rotation: $[\alpha]_{\text{D}}^{25} -14.1$ (c, 2 in H₂O)

Sigma: G1752

>>Derivative: TFA-Gly-L-Ile

Molecular Formula: C₁₀H₁₅F₃N₂O₄

Molecular Weight: 284.235

Accurate Mass: 284.098392

Percentage Composition: C 42.26%; H 5.32%; F 20.05%; N 9.86%; O 22.52%

Physical Description: Cryst. (AcOH/CH₂Cl₂)

Melting Point: Mp 175-177°

Optical Rotation: $[\alpha]_{\text{D}}^{22} +22.3$ (c, 0.85 in THF)

>>Derivative: TFA-Gly-L-Ile, Me ester

Molecular Formula: C₁₁H₁₇F₃N₂O₄

Molecular Weight: 298.261

Accurate Mass: 298.114042

Percentage Composition: C 44.30%; H 5.74%; F 19.11%; N 9.39%; O 21.46%

Physical Description: Cryst. (hexane)

Melting Point: Mp 72.5-73.5°

Optical Rotation: $[\alpha]_{\text{D}}^{26} -20.2$ (c, 1.1 in EtOH)

>>Variant: L-*allo*-form

Synonym(s): *N*-Glycyl-L-alloisoleucine

Molecular Formula: C₈H₁₆N₂O₃

Molecular Weight: 188.226

Accurate Mass: 188.116093

Percentage Composition: C 51.05%; H 8.57%; N 14.88%; O 25.50%

Optical Rotation: $[\alpha]_{\text{D}}^{25} -5.2$ (c, 2 in H₂O)

References:

Rao, K.R. *et al.*, *J. Biol. Chem.*, 1952, **198**, 507, (*synth*)

Weygand, F. *et al.*, *Chem. Ber.*, 1964, **97**, 1024, (*derivs*)