



Boiling Point: Bp_{0.75} 115°
Optical Rotation: $[\alpha]_{\text{D}}^{25}$ -23.4 (c, 1.95 in MeOH)
Density: d₄²⁰ 1.02
Refractive Index: n_D²⁰ 1.5006

>>Derivative: Amide

Synonym(s): α-Aminobenzenepropanamide, 9Cl. Phenylalanine amide

CAS Registry Number: 5241-59-8
Molecular Formula: C₉H₁₂N₂O
Molecular Weight: 164.207
Accurate Mass: 164.094963
Percentage Composition: C 65.83%; H 7.37%; N 17.06%; O 9.74%
Physical Description: Cryst. (C₆H₆)
Melting Point: Mp 91-93°
Optical Rotation: $[\alpha]_{\text{D}}^{24}$ -13.41 (MeOH)

>>Derivative: N-Formyl

CAS Registry Number: 59366-89-1
Molecular Formula: C₁₀H₁₁NO₃
Molecular Weight: 193.202
Accurate Mass: 193.073894
Percentage Composition: C 62.17%; H 5.74%; N 7.25%; O 24.84%
Physical Description: Plates (H₂O)
Melting Point: Mp 167°
Optical Rotation: $[\alpha]_{\text{D}}^{20}$ -75.2 (EtOH)

>>Derivative: N-Ac

CAS Registry Number: 10172-89-1
Molecular Formula: C₁₁H₁₃NO₃
Molecular Weight: 207.229
Percentage Composition: C 63.76%; H 6.32%; N 6.76%; O 23.16%
Melting Point: Mp 170-171°
Optical Rotation: $[\alpha]_{\text{D}}$ -49.3
Sigma: A3876

>>Derivative: N-Ac, Me ester

CAS Registry Number: 21156-62-7
Molecular Formula: C₁₂H₁₅NO₃
Molecular Weight: 221.255
Accurate Mass: 221.105194
Percentage Composition: C 65.14%; H 6.83%; N 6.33%; O 21.69%
Physical Description: Prisms (Et₂O)
Melting Point: Mp 90-91°
Optical Rotation: $[\alpha]_{\text{D}}^{25}$ -19 (c, 2 in MeOH)

>>Derivative: N-Ac, Et ester

CAS Registry Number: 20918-84-7
Molecular Formula: C₁₃H₁₇NO₃
Molecular Weight: 235.282
Accurate Mass: 235.120844
Percentage Composition: C 66.36%; H 7.28%; N 5.95%; O 20.40%
Physical Description: Cryst.
Melting Point: Mp 93.5-94.5°
Optical Rotation: $[\alpha]_{\text{D}}^{25}$ -61.8 (c, 1 in CHCl₃) (72% ee)

>>Derivative: N-Benzoyl

CAS Registry Number: 37002-52-1
Molecular Formula: C₁₆H₁₅NO₃
Molecular Weight: 269.299
Percentage Composition: C 71.36%; H 5.61%; N 5.20%; O 17.82%
Physical Description: Needles (H₂O)
Melting Point: Mp 154-155° (146-148°)
Optical Rotation: $[\alpha]$