



>>Variant: (S)-form

CAS Registry Number: 40856-44-8

Molecular Formula: C₉H₁₁NO₂

Molecular Weight: 165.191

Accurate Mass: 165.078979

Percentage Composition: C 65.44%; H 6.71%; N 8.48%; O 19.37%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 234-235°

Optical Rotation: [α]_D²⁵ −7.5 (H₂O)

>>Derivative: N-Me

Synonym(s): 3-(Methylamino)-3-phenylpropanoic acid

Molecular Formula: C₁₀H₁₃NO₂

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

Physical Description: Cryst. (MeOH/Et₂O)

Melting Point: Mp 162°

Optical Rotation: [α]_D −47 (c, 1.7 in MeOH)

>>Derivative: N-Ph

Synonym(s): 3-Anilino-3-phenylpropanoic acid

Molecular Formula: C₁₅H₁₅NO₂

Molecular Weight: 241.289

Accurate Mass: 241.110279

Percentage Composition: C 74.67%; H 6.27%; N 5.80%; O 13.26%

Physical Description: Solid

Melting Point: Mp 125-126°

>>Derivative: N-Ph, Me ester

Molecular Formula: C₁₆H₁₇NO₂

Molecular Weight: 255.316

Accurate Mass: 255.125929

Percentage Composition: C 75.27%; H 6.71%; N 5.49%; O 12.53%

Physical Description: Solid

Melting Point: Mp 113-114°

>>Variant: (±)-form

CAS Registry Number: 3646-50-2

Molecular Formula: C₉H₁₁NO₂

Molecular Weight: 165.191

Accurate Mass: 165.078979

Percentage Composition: C 65.44%; H 6.71%; N 8.48%; O 19.37%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 231°

Solubility: Sol. hot H₂O

>>Derivative: Hydrochloride

Physical Description: Prisms (EtOH)

Melting Point: Mp 218°

>>Derivative: Amide

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%

Melting Point: Mp 196-196.5 dec.°