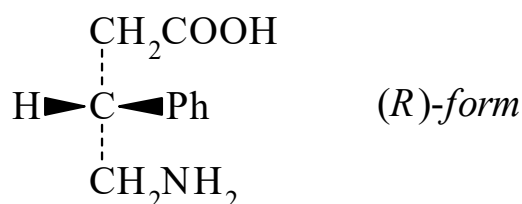




>>Entry Name: 4-Amino-3-phenylbutanoic acid

Synonym(s): β -(Aminomethyl)benzenepropanoic acid, 9CI. β -(Aminomethyl)hydrocinnamic acid, 8CI. β -PhenylGABA. Fenibut. Fenigam. Phenibut. Phenigam. Phenybut. Phenygam. Phenylgamma. PHG



CAS Registry Number: 1078-21-3

Related CAS Registry Numbers(s): 3060-41-1 35568-36-6 52950-37-5 52992-48-0

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%

Use/Importance: Mood elevator and tranquilliser

Calculated Log P Data: Log P -2.05 (calc)

Hazard & Toxicity: LD₅₀ (rat, ipr) 700 mg/kg

>>Variant: (R)-form

CAS Registry Number: 35568-36-6

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. (EtOH aq.)

Melting Point: Mp 149-152 dec.°

Boiling Point: Subl. 193-194°

Optical Rotation: [α]_D -6 (c, 2.5 in H₂O). [α]_D +2.3 (c, 1.3 in HCl aq., pH1)

>>Derivative: Me ester

Molecular Formula: C₁₁H₁₅NO₂

Molecular Weight: 193.245

Accurate Mass: 193.110279

Percentage Composition: C 68.37%; H 7.82%; N 7.25%; O 16.56%

Physical Description: Needles (MeOH/THF) (as hydrochloride)

Melting Point: Mp 170-171° (hydrochloride)

Optical Rotation: [α]_D²² +5.26 (c, 1.04 in MeOH)

>>Derivative: *N*-tert-Butoxycarbonyl

Molecular Formula: C₁₅H₂₁NO₄

Molecular Weight: 279.335

Accurate Mass: 279.147059

Percentage Composition: C 64.50%; H 7.58%; N 5.01%; O 22.91%

Physical Description: Cryst. (Et₂O/pentane)

Melting Point: Mp 106-107°

Optical Rotation: [α]_D²² +7.78 (c, 1.08 in MeOH)

>>Variant: (S)-form

CAS Registry Number: 62596-63-8

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. (Et₂O/EtOH aq.)

Melting Point: Mp 213-214°

Optical Rotation: [α]_D²⁰ +12.9 (c, 1.11 in H₂O). [α]_D -2.4 (c, 1.3 in HCl aq., pH1)