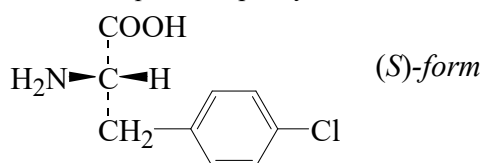




>>Entry Name: **2-Amino-3-(4-chlorophenyl)propanoic acid**

Synonym(s): 4-Chlorophenylalanine, 9Cl. 3-(*p*-Chlorophenyl)alanine, 8Cl. *p*-Chlorophenylalanine. **Fenclonine**, INN, USAN. CP 10188. NSC 77370



CAS Registry Number: 1991-78-2

Related CAS Registry Numbers(s): 14091-08-8 23434-91-5 33965-47-8 132210-40-3

Molecular Formula: C₉H₁₀ClNO₂

Molecular Weight: 199.636

Accurate Mass: 199.040006

Percentage Composition: C 54.15%; H 5.05%; Cl 17.76%; N 7.02%; O 16.03%

Use/Importance: 5-HT antagonist, causes 5-HT depletion in brain by binding irreversibly to tryptophan hydroxylase

Aldrich: 28252-9

Fluka: 25920

Sigma: C8655

>>Variant: (*S*)-form

Synonym(s): L-form

CAS Registry Number: 14173-39-8

Molecular Formula: C₉H₁₀ClNO₂

Molecular Weight: 199.636

Accurate Mass: 199.040006

Percentage Composition: C 54.15%; H 5.05%; Cl 17.76%; N 7.02%; O 16.03%

Melting Point: Mp 255-256°. Mp 263° (dec.)

Optical Rotation: [α]_D²⁰ -24 (c, 1 in H₂O). [α]_D²⁰ +2.5 (c, 1 in 1M HCl) (>=95.5% ee)

>>Derivative: Me ester

CAS Registry Number: 14173-40-1

Molecular Formula: C₁₀H₁₂ClNO₂

Molecular Weight: 213.663

Accurate Mass: 213.055656

Percentage Composition: C 56.21%; H 5.66%; Cl 16.59%; N 6.56%; O 14.98%

Physical Description: Cryst. (MeOH/Et₂O) (as hydrochloride)

Melting Point: Mp 186-189° (177-178°) (hydrochloride)

>>Derivative: Et ester

CAS Registry Number: 52031-05-7

Molecular Formula: C₁₁H₁₄ClNO₂

Molecular Weight: 227.69

Accurate Mass: 227.071306

Percentage Composition: C 58.03%; H 6.20%; Cl 15.57%; N 6.15%; O 14.05%

Physical Description: Cryst. (as hydrochloride)

Melting Point: Mp 168-170° (hydrochloride)

>>Variant: (±)-form

CAS Registry Number: 7424-00-2

Molecular Formula: C₉H₁₀ClNO₂

Molecular Weight: 199.636

Accurate Mass: 199.040006

Percentage Composition: C 54.15%; H 5.05%; Cl 17.76%; N 7.02%; O 16.03%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 238-240°

Calculated Log P Data: Log P -0.84 (uncertain value) (calc)

Other Data: Dec. with yellowing from 223°

Aldrich: 13071-0

Sigma: C6506