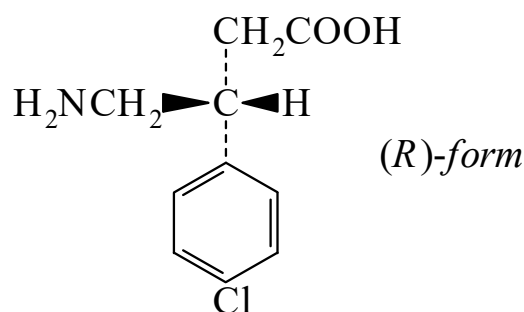




>>Entry Name: **Baclofen**, BAN, INN, JAN, USAN

Synonym(s): β -(Aminomethyl)-4-chlorobenzenepropanoic acid, 9Cl. β -(Aminomethyl)-*p*-chlorohydrocinnamic acid, 8Cl. 4-Amino-3-(4-chlorophenyl)butanoic acid. Gabalon. Lioresal. Spastin. Ba 34647. C 34647Ba. Baclon



CAS Registry Number: 1134-47-0

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%

Use/Importance: Skeletal muscle relaxant, GABA_B agonist

Hazard & Toxicity: LD₅₀ (rat, orl) 145 mg/kg

Sigma: B5399

>>Variant: (*R*)-form

CAS Registry Number: 69308-37-8

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. (EtOH/Et₂O) (as hydrochloride)

Melting Point: Mp 215° (hydrochloride)

Optical Rotation: [α]_D²⁰ -2 (c, 0.2 in H₂O)

Other Data: More active enantiomer

>>Variant: (*S*)-form

CAS Registry Number: 66514-99-6

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%

Melting Point: Mp 215° (as hydrochloride)

Optical Rotation: [α]_D +2 (c, 0.2 in H₂O)

>>Variant: ($\pm$)-form

CAS Registry Number: 62594-36-9

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. (H₂O)

Melting Point: Mp 206-208°

Calculated Log P Data: Log P -1.33 (calc)

References: