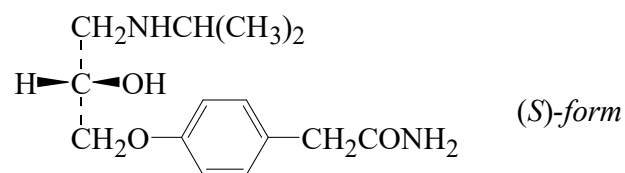




>>Entry Name: Atenolol, BAN, INN, JAN, USAN

Synonym(s): 4-[2-Hydroxy-3-[(1-methylethyl)amino]propoxy]benzeneacetamide, 9CI. Atenix. Atenol. Cuxanorm. Myocord. Prenormin. Selobloc. Tenoblock. Tenoretic. Tenormin. Totamol. Vasaten. ICI 66082. Many other names



CAS Registry Number: 29122-68-7

Molecular Formula: C₁₄H₂₂N₂O₃

Molecular Weight: 266.339

Accurate Mass: 266.163043

Percentage Composition: C 63.14%; H 8.33%; N 10.52%; O 18.02%

Biological Use/Importance: β-Adrenergic blocker, antihypertensive agent

Development Status: Marketed drug. Approved 1981

Calculated Log P Data: Log P -0.11 (calc)

Hazard & Toxicity: Human and exp. reprod. effects. LD₅₀ (rat, orl) 3000 mg/kg

Sigma: A7655

>>Variant: (*R*)-form

CAS Registry Number: 56715-13-0

Molecular Formula: C₁₄H₂₂N₂O₃

Molecular Weight: 266.339

Accurate Mass: 266.163043

Percentage Composition: C 63.14%; H 8.33%; N 10.52%; O 18.02%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 151.5-152.8°

Optical Rotation: [α]_D²⁵+12.53 (c, 0.9 in EtOH) (>97% ee)

Aldrich: 33088-4

>>Variant: (*S*)-form

Synonym(s): Esatenolol

CAS Registry Number: 93379-54-5

Molecular Formula: C₁₄H₂₂N₂O₃

Molecular Weight: 266.339

Accurate Mass: 266.163043

Percentage Composition: C 63.14%; H 8.33%; N 10.52%; O 18.02%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 151-152.5°

Optical Rotation: [α]_D²⁵-13.1 (c, 0.9 in EtOH) (>99% ee)

Other Data: Pharmacol. active isomer

Aldrich: 33089-2

>>Variant: (±)-form

CAS Registry Number: 60966-51-0

Molecular Formula: C₁₄H₂₂N₂O₃

Molecular Weight: 266.339

Accurate Mass: 266.163043

Percentage Composition: C 63.14%; H 8.33%; N 10.52%; O 18.02%

Melting Point: Mp 146-148°

References: