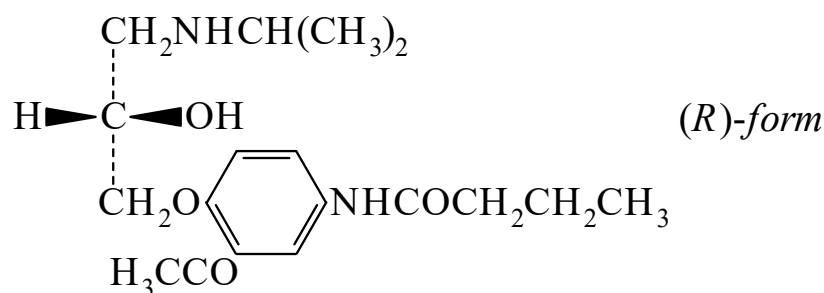




>>Entry Name: **Acebutolol**, BAN, INN, USAN

Synonym(s): *N*-[3-Acetyl-4-[2-hydroxy-3-[(1-methylethyl)amino]propoxy]phenyl]butanamide, 9Cl. 3'-Acetyl-4'-[2-hydroxy-3-(isopropylamino)propoxy]butyranilide, 8Cl. 1-(2-Acetyl-4-butyramidophenoxy)-2-hydroxy-3-isopropylaminopropane



CAS Registry Number: 28197-63-9

Molecular Formula: C₁₈H₂₈N₂O₄

Molecular Weight: 336.43

Accurate Mass: 336.204908

Percentage Composition: C 64.26%; H 8.39%; N 8.33%; O 19.02%

Use/Importance: β-Adrenoceptor antagonist

Calculated Log P Data: Log P 1.63 (calc)

>>Variant: (*R*)-form

CAS Registry Number: 68107-81-3

Molecular Formula: C₁₈H₂₈N₂O₄

Molecular Weight: 336.43

Accurate Mass: 336.204908

Percentage Composition: C 64.26%; H 8.39%; N 8.33%; O 19.02%

>>Derivative: Hydrochloride

CAS Registry Number: 96450-13-4

Optical Rotation: [α]_D³⁰+12

>>Variant: (±)-form

CAS Registry Number: 37517-30-9

Molecular Formula: C₁₈H₂₈N₂O₄

Molecular Weight: 336.43

Accurate Mass: 336.204908

Percentage Composition: C 64.26%; H 8.39%; N 8.33%; O 19.02%

Physical Description: Cryst.

Melting Point: Mp 119-123°

Hazard & Toxicity: Human reprod. and teratogenic effects

>>Derivative: Hydrochloride

Synonym(s): Acebutolol hydrochloride, JAN, USAN. M & B 17803A. IL-17803A

CAS Registry Number: 34381-68-5

Physical Description: Cryst. (MeOH/Et₂O)

Melting Point: Mp 141-143°

Hazard & Toxicity: Exp. reprod. and teratogenic effects

Sigma: A3669

References:

Basil, B. *et al.*, *J. Med. Chem.*, 1976, **19**, 399, (*synth*)

Nelson, W.L. *et al.*, *J.O.C.*, 1978, **43**, 4907, (*cd*)

Carpy, A. *et al.*, *Acta Cryst. B*, 1979, **35**, 185, (*cryst struct*)

Basil, B. *et al.*, *Pharmacol. Hypertens. Drugs*, 1980, 283, (*pharmacol*)

Singh, B.N. *et al.*, *Drugs*, 1985, **29**, 531, (*rev*)

Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, 1987, 5024, (*synonyms*)

Foster, R.T. *et al.*, *Anal. Profiles Drug Subst.*, 1990, **19**, 1, (*rev*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 628

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, AAE100; AAE125