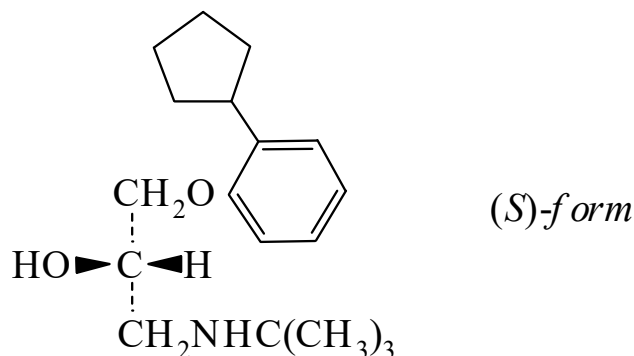




>>Entry Name: Penbutolol, BAN, INN

Synonym(s): 1-(2-Cyclopentylphenoxy)-3-[(1,1-dimethylethyl)amino]-2-propanol, 9Cl. 3-*tert*-Butylamino-1-(2-cyclopentylphenoxy)-2-propanol. Terbuclomine. Hoe 39893d



Molecular Formula: C₁₈H₂₉NO₂

Molecular Weight: 291.433

Accurate Mass: 291.219829

Percentage Composition: C 74.18%; H 10.03%; N 4.81%; O 10.98%

Use/Importance: β-Adrenergic blocker

Calculated Log P Data: Log P 4.04 (calc)

>>Variant: (S)-form

CAS Registry Number: 38363-40-5

Molecular Formula: C₁₈H₂₉NO₂

Molecular Weight: 291.433

Accurate Mass: 291.219829

Percentage Composition: C 74.18%; H 10.03%; N 4.81%; O 10.98%

Hazard & Toxicity: LD₅₀ (rat, orl) 1265 mg/kg. Nongenotoxic

>>Derivative: Hydrochloride

CAS Registry Number: 28291-30-7

Melting Point: Mp 92-93°

Optical Rotation: [α]_D²⁰ -26.4 (c, 1 in MeOH)

>>Derivative: Sulfate (2:1)

Synonym(s): Penbutolol sulfate, JAN, USAN. Betapressin. Blocotin. Hostabloc. Ipobar. Lesipressin. Hoe 893d

CAS Registry Number: 38363-32-5

Melting Point: Mp 216-218 dec.°

Optical Rotation: [α]_D²⁰ -24.6 (c, 1 in MeOH)

Hazard & Toxicity: LD₅₀ (rat, orl) 1350 mg/kg

References:

Lessenich, H. *et al.*, *Arzneim.-Forsch.*, 1972, **22**, 930, (*synth, pharmacol*)

Vallner, J.J. *et al.*, *J. Clin. Pharmacol.*, 1977, **17**, 231, (*pharmacol*)

Hajdu, P. *et al.*, *Arzneim.-Forsch.*, 1979, **29**, 602, (*props*)

Kaiser, J. *et al.*, *Arzneim.-Forsch.*, 1980, **30**, 420, (*pharmacol*)

Leger, M. *et al.*, *Mol. Pharmacol.*, 1980, **17**, 339, (*cryst struct*)

Heel, R.C. *et al.*, *Drugs*, 1981, **22**, 1, (*rev*)

Kan, K. *et al.*, *Agric. Biol. Chem.*, 1985, **49**, 207, (*synth*)

Kuhnert-Brandstaetter, M. *et al.*, *Sci. Pharm.*, 1987, **55**, 13, (*polymorphism*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 637

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, PAP225; PAP230