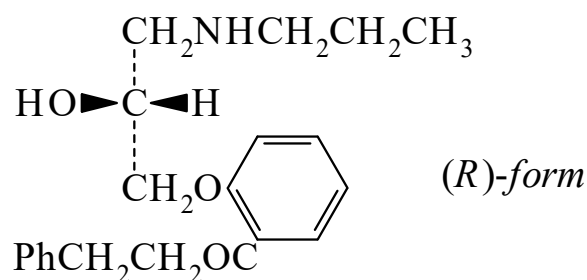




>>Entry Name: Propafenone, BAN, INN

Synonym(s): 1-[2-[2-Hydroxy-3-(propylamino)propoxy]phenyl]-3-phenyl-1-propanone, 9Cl. 2'-(2-Hydroxy-3-propylaminopropoxy)-3-phenylpropiophenone, 8Cl. Fenopraïne



CAS Registry Number: 54063-53-5

Molecular Formula: C₂₁H₂₇NO₃

Molecular Weight: 341.449

Accurate Mass: 341.199094

Percentage Composition: C 73.87%; H 7.97%; N 4.10%; O 14.06%

Biological Use/Importance: β-Adrenergic receptor antagonist. Coronary vasodilator. Antiarrhythmic (Class Ic) agent used for the management of ventricular and supraventricular arrhythmias

Development Status: Approved 1989

Calculated Log P Data: Log P 3.42 (calc)

Hazard & Toxicity: LD₅₀ (mus, orl) 440 mg/kg

Sigma: P4670

>>Variant: (R)-form

CAS Registry Number: 107381-31-7

Molecular Formula: C₂₁H₂₇NO₃

Molecular Weight: 341.449

Accurate Mass: 341.199094

Percentage Composition: C 73.87%; H 7.97%; N 4.10%; O 14.06%

Physical Description: Cryst. (petrol)

Melting Point: Mp 65°

Optical Rotation: [α]_{Hg365}²⁰ -19.6 (c, 1.02 in EtOH) (98.8% ee)

>>Derivative: Hydrochloride

CAS Registry Number: 107381-35-1

Physical Description: Cryst. (EtOH)

Melting Point: Mp 172-174°

Optical Rotation: [α]_{Hg546}²² +8.2 (c, 0.97 in MeOH)

Sigma: P9833

>>Variant: (S)-form

CAS Registry Number: 107381-32-8

Molecular Formula: C₂₁H₂₇NO₃

Molecular Weight: 341.449

Accurate Mass: 341.199094

Percentage Composition: C 73.87%; H 7.97%; N 4.10%; O 14.06%

Physical Description: Cryst. (petrol)

Melting Point: Mp 65°

Optical Rotation: [α]_{Hg365}²⁰ +18.7 (c, 1.08 in EtOH) (97.6% ee)

Other Data: More pharmacol. active isomer

>>Derivative: Hydrochloride

CAS Registry Number: 107381-36-2

Physical Description: Cryst. (EtOH)

Melting Point: Mp 172-174°

Optical Rotation: [α]_{Hg546}²¹ -8.5 (c, 1 in MeOH)

Sigma: P9708