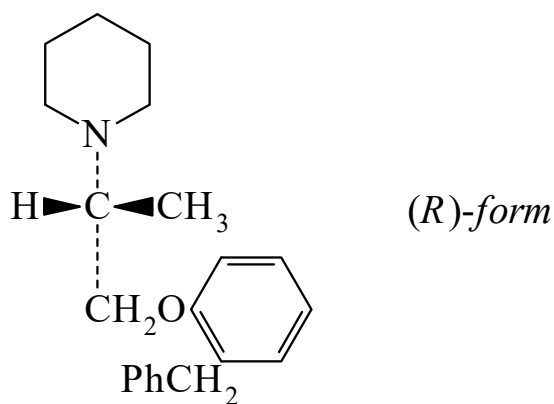




>>Entry Name: Benproperine, INN

Synonym(s): 1-[1-Methyl-2-[2-(phenylmethyl)phenoxy]ethyl]piperidine, 9Cl. 1-[1-Methyl-2-[(α -phenyl-*o*-tolyl)oxy]ethyl]piperidine, 8Cl. 1-[2-(2-Benzylphenoxy)-1-methylethyl]piperidine



CAS Registry Number: 2156-27-6

Related CAS Registry Numbers(s): 3563-76-6 19428-14-9 64238-92-2

Molecular Formula: C₂₁H₂₇NO

Molecular Weight: 309.45

Accurate Mass: 309.209264

Percentage Composition: C 81.51%; H 8.79%; N 4.53%; O 5.17%

Use/Importance: Antitussive agent

Boiling Point: Bp_{0.25} 164-167°

Calculated Log P Data: Log P 5.79 (calc)

Hazard & Toxicity: LD₅₀ (mus, orl) 1087 mg/kg. Exp. reprod. effects

>>Variant: (*R*)-form

CAS Registry Number: 124678-30-4

Molecular Formula: C₂₁H₂₇NO

Molecular Weight: 309.45

Accurate Mass: 309.209264

Percentage Composition: C 81.51%; H 8.79%; N 4.53%; O 5.17%

>>Derivative: Phosphate

CAS Registry Number: 124678-31-5

Physical Description: Cryst. (EtOH)

Melting Point: Mp 164-168°

Optical Rotation: [α]_D²⁰ +22.7 (c, 1.05 in EtOH) (98% ee)

>>Variant: (*S*)-form

CAS Registry Number: 124700-66-9

Molecular Formula: C₂₁H₂₇NO

Molecular Weight: 309.45

Accurate Mass: 309.209264

Percentage Composition: C 81.51%; H 8.79%; N 4.53%; O 5.17%

>>Derivative: Phosphate

CAS Registry Number: 124700-67-0

Physical Description: Cryst.

Melting Point: Mp 162-165°

Optical Rotation: [α]_D²⁵ -17.4 (c, 1.10 in EtOH) (87% ee)

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

CAS Registry Number: 138663-99-7

Molecular Formula: C₂₁H₂₇NO

Molecular Weight: 309.45

Accurate Mass: 309.209264

Percentage Composition: C 81.51%; H 8.79%; N 4.53%; O 5.17%