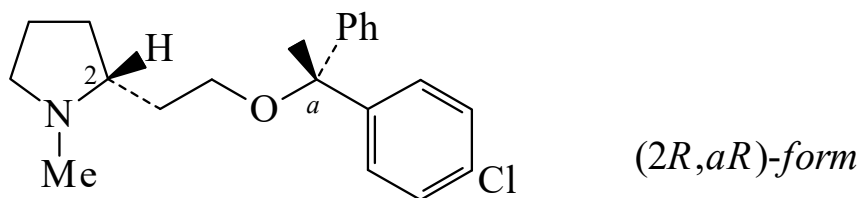




>>Entry Name: Clemastine, BAN, INN, USAN

Synonym(s): 2-[2-[1-(4-Chlorophenyl)-1-phenylethoxy]ethyl]-1-methylpyrrolidine, 9Cl. 2-[[2-(*p*-Chloro- α -methyl- α -phenylbenzyl)oxy]ethyl]-1-methylpyrrolidine, 8Cl. Meclastine. Mecloprodine. Many other names



Molecular Formula: C₂₁H₂₆ClNO

Molecular Weight: 343.895

Accurate Mass: 343.170291

Percentage Composition: C 73.35%; H 7.62%; Cl 10.31%; N 4.07%; O 4.65%

Use/Importance: Histamine H₁-receptor antagonist

>>Variant: (2*R*, α *R*)-form

CAS Registry Number: 15686-51-8

Molecular Formula: C₂₁H₂₆ClNO

Molecular Weight: 343.895

Accurate Mass: 343.170291

Percentage Composition: C 73.35%; H 7.62%; Cl 10.31%; N 4.07%; O 4.65%

Physical Description: Cryst. (hexane)

Melting Point: Mp 58-61°

Boiling Point: Bp_{0.02} 155°

Optical Rotation: $[\alpha]_D^{20} +33.6$ (c, 2 in EtOH)

Other Data: Pharmacol. active isomer

>>Derivative: Fumarate (1:1)

Synonym(s): Clemastine fumarate, JAN, USAN. Tavegil. Lactetin

CAS Registry Number: 14976-57-9

Physical Description: Cryst. (MeOH)

Melting Point: Mp 177-178 dec.°

Optical Rotation: $[\alpha]_D^{20} +16.9$ (c, 2 in MeOH)

Hazard & Toxicity: LD₅₀ (rat, orl) 3550 mg/kg

Sigma: C8903

>>Variant: (2*R*, α *S*)-form

CAS Registry Number: 61826-31-1

Molecular Formula: C₂₁H₂₆ClNO

Molecular Weight: 343.895

Accurate Mass: 343.170291

Percentage Composition: C 73.35%; H 7.62%; Cl 10.31%; N 4.07%; O 4.65%

Boiling Point: Bp_{0.02} 155°

Optical Rotation: $[\alpha]_D +58.2$ (c, 2 in EtOH)

>>Derivative: Fumarate (1:1)

CAS Registry Number: 61826-32-2

Physical Description: Cryst. (MeOH)

Melting Point: Mp 159-160°

Optical Rotation: $[\alpha]_D +32.6$ (c, 2 in MeOH)

References: