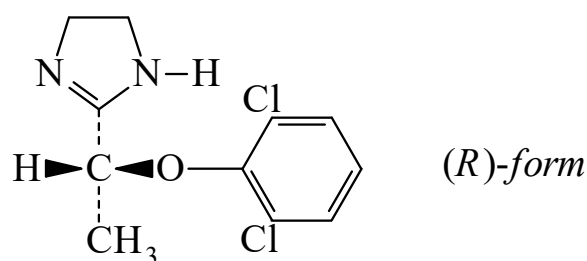




>>Entry Name: Lofexidine, BAN, INN

Synonym(s): 2-[1-(2,6-Dichlorophenoxy)ethyl]-4,5-dihydro-1*H*-imidazole, 9Cl. 2-[(2,6-Dichlorophenoxy)ethyl]-2-imidazoline, 8Cl



CAS Registry Number: 31036-80-3

Related CAS Registry Numbers(s): 21498-08-8

Molecular Formula: C₁₁H₁₂Cl₂N₂O

Molecular Weight: 259.134

Accurate Mass: 258.032667

Percentage Composition: C 50.99%; H 4.67%; Cl 27.36%; N 10.81%; O 6.17%

Use/Importance: α -Adrenoceptor agonist. Antihypertensive

Calculated Log P Data: Log P 3.6 (calc)

Hazard & Toxicity: LD₅₀ (rat, orl) 70 mg/kg. Exp. reprod. and teratogenic effects

>>Variant: (*R*)-form

Synonym(s): Levlofexidine, INN

CAS Registry Number: 81447-78-1

Molecular Formula: C₁₁H₁₂Cl₂N₂O

Molecular Weight: 259.134

Accurate Mass: 258.032667

Percentage Composition: C 50.99%; H 4.67%; Cl 27.36%; N 10.81%; O 6.17%

Physical Description: Cryst.

Melting Point: Mp 126-127°

Optical Rotation: $[\alpha]_D^{20} -90$ (c, 1 in EtOH)

>>Derivative: Hydrochloride

CAS Registry Number: 87038-06-0

Melting Point: Mp 229-230°

Optical Rotation: $[\alpha]_D^{20} -33.2$ (c, 1 in EtOH)

>>Variant: (*S*)-form

Synonym(s): Dexlofexidine, INN

CAS Registry Number: 81447-79-2

Molecular Formula: C₁₁H₁₂Cl₂N₂O

Molecular Weight: 259.134

Accurate Mass: 258.032667

Percentage Composition: C 50.99%; H 4.67%; Cl 27.36%; N 10.81%; O 6.17%

Physical Description: Cryst.

Melting Point: Mp 125-126°

Optical Rotation: $[\alpha]_D^{20} +73.7$ (c, 1 in EtOH)

>>Derivative: Hydrochloride

CAS Registry Number: 87858-98-8

Melting Point: Mp 236-237°

Optical Rotation: $[\alpha]_D^{20} +33.4$ (c, 1 in EtOH)

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