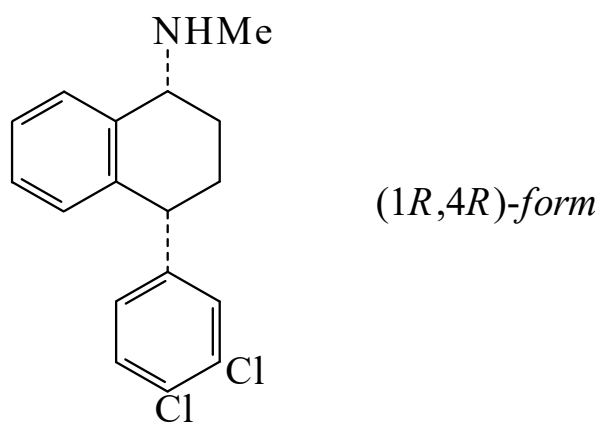




>>Entry Name: Sertraline, BAN, INN

Synonym(s): 4-(3,4-Dichlorophenyl)-1,2,3,4-tetrahydro-*N*-methyl-1-naphthalenamine, 9Cl



Related CAS Registry Numbers(s): 79617-89-3 79617-95-1

Molecular Formula: C₁₇H₁₇Cl₂N

Molecular Weight: 306.233

Accurate Mass: 305.073803

Percentage Composition: C 66.68%; H 5.60%; Cl 23.15%; N 4.57%

Biological Use/Importance: Selectively inhibits re-uptake of 5HT. Antidepressant

Calculated Log P Data: Log P 5.35 (calc)

>>Variant: (1*R*,4*R*)-form

Synonym(s): (–)-*cis*-form

CAS Registry Number: 79617-98-4

Molecular Formula: C₁₇H₁₇Cl₂N

Molecular Weight: 306.233

Accurate Mass: 305.073803

Percentage Composition: C 66.68%; H 5.60%; Cl 23.15%; N 4.57%

>>Derivative: Hydrochloride

CAS Registry Number: 79645-15-1

Melting Point: Mp 243-245°

Optical Rotation: $[\alpha]_{\text{D}}^{23} -37.2$ (c, 2.0 in MeOH)

>>Variant: (1*R*,4*S*)-form

Synonym(s): (+)-*trans*-form

CAS Registry Number: 91797-60-3

Molecular Formula: C₁₇H₁₇Cl₂N

Molecular Weight: 306.233

Accurate Mass: 305.073803

Percentage Composition: C 66.68%; H 5.60%; Cl 23.15%; N 4.57%

>>Derivative: Hydrochloride

CAS Registry Number: 79896-31-4

Physical Description: Cryst. (MeOH/Et₂O)

Melting Point: Mp 255-257°

Optical Rotation: $[\alpha]_{\text{D}}^{22} +41$ (MeOH)

>>Variant: (1*S*,4*R*)-form

Synonym(s): (–)-*trans*-form

CAS Registry Number: 79951-46-5

Molecular Formula: C₁₇H₁₇Cl₂N

Molecular Weight: 306.233

Accurate Mass: 305.073803

Percentage Composition: C 66.68%; H 5.60%; Cl 23.15%; N 4.57%

>>Derivative: Hydrochloride

CAS Registry Number: 79896-32-5

Physical Description: Cryst. (MeOH/Et₂O)

Melting Point: Mp 257-258°

Optical Rotation: $[\alpha]$