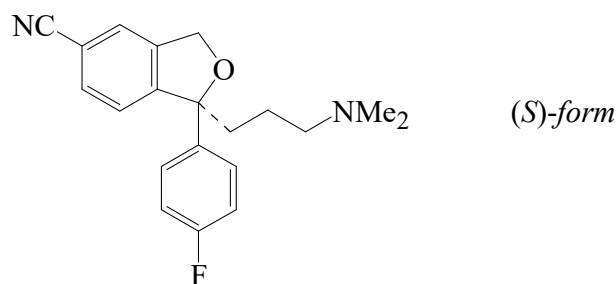




>>Entry Name: Citalopram, BAN, INN

Synonym(s): 1-[3-(Dimethylamino)propyl-1-(4-fluorophenyl)]-1,3-dihydro-5-isobenzofurancarbonitrile, 9Cl. 1-(3-Dimethylaminopropyl)-1-(4-fluorophenyl)-5-cyanophthalan. Cipramil. Nitalapram. Lu 10-171



CAS Registry Number: 59729-33-8

Molecular Formula: C₂₀H₂₁FN₂O

Molecular Weight: 324.397

Accurate Mass: 324.163791

Percentage Composition: C 74.05%; H 6.52%; F 5.86%; N 8.64%; O 4.93%

Biological Use/Importance: 5HT re-uptake inhibitor. Antidepressant

Development Status: Launched 1989

Sigma: C1206

>>Variant: (*R*)-form

CAS Registry Number: 128196-02-1

Molecular Formula: C₂₀H₂₁FN₂O

Molecular Weight: 324.397

Accurate Mass: 324.163791

Percentage Composition: C 74.05%; H 6.52%; F 5.86%; N 8.64%; O 4.93%

Physical Description: Oil

Optical Rotation: [α]_D -12.34 (c, 1 in MeOH)

>>Derivative: Oxalate

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 147-148°

Optical Rotation: [α]_D -12.08 (c, 1 in MeOH)

>>Variant: (*S*)-form

Synonym(s): Escitalopram, INN

CAS Registry Number: 128196-01-0

Molecular Formula: C₂₀H₂₁FN₂O

Molecular Weight: 324.397

Accurate Mass: 324.163791

Percentage Composition: C 74.05%; H 6.52%; F 5.86%; N 8.64%; O 4.93%

Biological Use/Importance: Antidepressant

Physical Description: Oil

Optical Rotation: [α]_D +11.81 (c, 1 in MeOH)

Other Data: Pharmacol. active isomer

>>Derivative: Oxalate

Synonym(s): Escitalopram oxalate, USAN

CAS Registry Number: 219861-08-2

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 147-148°

Optical Rotation: [α]_D +12.31 (c, 1 in MeOH)

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

CAS Registry Number: 128196-03-2

Molecular Formula: C₂₀H₂₁FN₂O

Molecular Weight: 324.397

Accurate Mass: 324.163791

Percentage Composition: C 74.05%; H 6.52%; F 5.86%; N 8.64%; O 4.93%

Calculated Log P Data: Log P 3.47 (uncertain value) (calc)