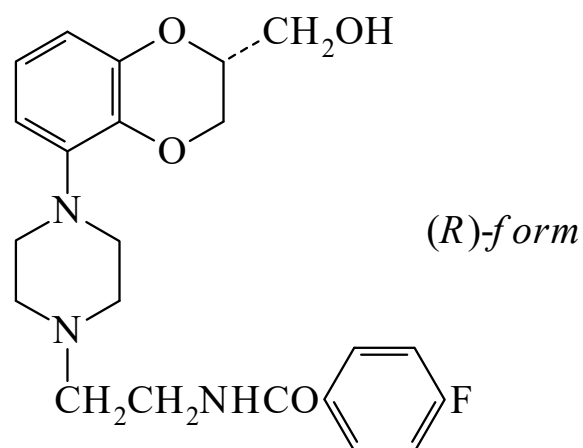




>>Entry Name: Flesinoxan, INN

Synonym(s): *N*-[2-[4-[2,3-Dihydro-2-(hydroxymethyl)-1,4-benzodioxin-5-yl]-1-piperazinyl]ethyl]-4-fluorobenzamide, 9CI



CAS Registry Number: 98205-86-8

Related CAS Registry Numbers(s): 132741-86-7

Molecular Formula: C₂₂H₂₆FN₃O₄

Molecular Weight: 415.463

Accurate Mass: 415.190735

Percentage Composition: C 63.60%; H 6.31%; F 4.57%; N 10.11%; O 15.40%

Use/Importance: Selective 5-HT_{1A}-receptor agonist. Antihypertensive agent. Potential antidepressant

Calculated Log P Data: Log P 2.87 (calc)

>>Variant: (*R*)-form

CAS Registry Number: 98206-10-1

Molecular Formula: C₂₂H₂₆FN₃O₄

Molecular Weight: 415.463

Accurate Mass: 415.190735

Percentage Composition: C 63.60%; H 6.31%; F 4.57%; N 10.11%; O 15.40%

Optical Rotation: [α]_D +26 (c, 1 in MeOH) (>97% ee)

>>Derivative: Hydrochloride

Synonym(s): DU 29373

CAS Registry Number: 98205-89-1

Physical Description: Cryst. (EtOH/Et₂O)

Melting Point: Mp 183-184°. Mp 187-188°

Optical Rotation: [α]_D +25 (c, 1 in MeOH)

>>Variant: (*S*)-form

CAS Registry Number: 145167-51-7

Molecular Formula: C₂₂H₂₆FN₃O₄

Molecular Weight: 415.463

Accurate Mass: 415.190735

Percentage Composition: C 63.60%; H 6.31%; F 4.57%; N 10.11%; O 15.40%

Optical Rotation: [α]_D -27 (c, 1 in MeOH) (>98% ee)

>>Derivative: Hydrochloride

CAS Registry Number: 145167-52-8

Physical Description: Cryst. (EtOH/Et₂O)

Melting Point: Mp 183-184.5°

Optical Rotation: [α]_D -24 (c, 1 in MeOH)

References:

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