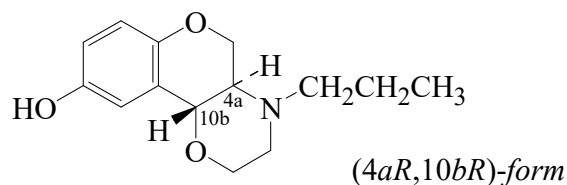




>>Entry Name: 3,4,4a,10b-Tetrahydro-4-propyl-2H,5H[1]benzopyrano[4,3-b]-1,4-oxazin-9-ol, 9CI

Synonym(s): PD 128907



Related CAS Registry Numbers(s): 123594-64-9

Molecular Formula: C₁₄H₁₉NO₃

Molecular Weight: 249.309

Accurate Mass: 249.136494

Percentage Composition: C 67.45%; H 7.68%; N 5.62%; O 19.25%

Biological Use/Importance: Dopamine D₃ receptor agonist

>>Variant: (4aR,10bR)-form

CAS Registry Number: 123671-92-1

Molecular Formula: C₁₄H₁₉NO₃

Molecular Weight: 249.309

Accurate Mass: 249.136494

Percentage Composition: C 67.45%; H 7.68%; N 5.62%; O 19.25%

Physical Description: Solid (EtOH)

Melting Point: Mp 265-271° (dec.) (as hydrochloride)

Optical Rotation: [α]_D +62.7 (c, 1.07 in H₂O) (as hydrochloride)

Other Data: Pharmacol. active isomer

>>Variant: (4aS,10bS)-form

CAS Registry Number: 123671-93-2

Molecular Formula: C₁₄H₁₉NO₃

Molecular Weight: 249.309

Accurate Mass: 249.136494

Percentage Composition: C 67.45%; H 7.68%; N 5.62%; O 19.25%

Melting Point: Mp 259-264° (dec.) (as hydrochloride)

Optical Rotation: [α]_D -63 (c, 1.11 in H₂O) (as hydrochloride)

>>Variant: (4aRS,10bRS)-form

Synonym(s): (±)-trans-form

CAS Registry Number: 112960-12-0

Molecular Formula: C₁₄H₁₉NO₃

Molecular Weight: 249.309

Accurate Mass: 249.136494

Percentage Composition: C 67.45%; H 7.68%; N 5.62%; O 19.25%

Physical Description: Oil

>>Derivative: Hydrochloride

CAS Registry Number: 112960-16-4

Physical Description: Cryst. (EtOH/Et₂O)

Melting Point: Mp 220° (dec.)

pKa Value: pK_a 6.1; pK_a 10.3

References:

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Dijkstra, D. *et al.*, *J. Med. Chem.*, 1988, **31**, 2178-2182, ((±)-trans-form, *synth*, *pmr*, *ir*, *pharmacol*)
DeWald, H.A. *et al.*, *J. Med. Chem.*, 1990, **33**, 445-450, (*isomers*, *synth*, *pmr*, *pharmacol*)
Pugsley, T.A. *et al.*, *J. Pharmacol. Exp. Ther.*, 1995, **275**, 1355-1366, (*pharmacol*)
Bristow, L.J. *et al.*, *Neuropharmacology*, 1996, **35**, 285-294, (*pharmacol*)
Khroyan, T.V. *et al.*, *Behav. Pharmacol.*, 1997, **8**, 65-74, (*pharmacol*)