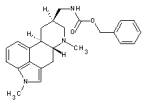

Formula: C25H29N3O2

MW: 403.52

CAS: 17692-51-2

TNP NUMBER: TNP00153

MDL NUMBER: MFCD00153829

Smiles: C1[C@@H](C[C@H]2([C@H](N1C)Cc1c3c(n(c1)C)cccc23))CNC(OCc1ccccc1)=O

ACCEPTORS: 2

DONORS: 1

ROTATION BONDS: 3

N+O: 5

Chiral Centers: 3

LogP: 6.12

LogS: -5.81

LIPINSKI: 3

Synonyms:
N-CBZ-[(8BETA)-1,6-DIMETHYLERGOLIN-8-YL]METHYLAMINE;METERGOLINE;METERGOLINE PHENYLMETHYL
ESTER;[((8BETA)-1,6-DIMETHYLERGOLIN-8-YL)METHYL]CARBAMIC ACID PHENYLMETHYL
ESTER;(((8-beta)-1,6-dimethylergolin-8-yl)methyl)-carbamicacibenzylester;(((8-beta)-1,6-dimethylergolin-8-yl)methyl)-carbamicaciphenylmethylest;((1,6-dimethylergolin-8-beta-yl)methyl)-carbamicacibenzylester;1,6-dimethyl-8-beta-carbobenzyloxaminomethyl-10-alpha-ergoline

CAS:17692-51-2

MF:C25H29N3O2

MW:403.52

EINECS:241-686-3

Product Categories:Serotonin receptor METERGOLINE

Chemical Properties: mp 148-150 C(lit.) storage temp. -20C solubility 0.1 M HCl: 1.4 mg/mL Merck 13,5962

CAS DataBase Reference: 17692-51-2(

CAS DataBase Reference:) Xn Risk Statements 20/21/22 Safety Statements 36 WGK Germany 3 RTECS FA1070000 METERGOLINE

Usage And Synthesis: Biological ActivityAntagonist at 5-HT 1 /5-HT 2 with activity at 5-HT 1D . Has moderate affinity for 5-HT 6 and high affinity for 5-HT 7 . METERGOLINE