



Formula: C₂₃H₂₅BrN₂O₃

MW: 457.37

MDL: MFCD00731295

TNP: TNP00035



LogP: 5.1

LogS: -5.3

Acceptors: 3

Donors: 2

Rotation Bonds: 3

Chiral Centers: 1

N+O: 5

LIPINSKY: 4

IUPAC: 11-(2-bromo-3,6-dimethoxyphenyl)-3,3-dimethyl-2,3,4-trihydro-5H,10H,11H-benzo[b]benzo[2,1-f]1,4-diazepin-1-one

Smiles: C=12C(c3c(c(OC)ccc3OC)Br)Nc3ccccc3NC1CC(CC2=O)(C)C