



Formula: C₁₆H₁₈BrNO₄

MW: 368.23

CAS: 16659-88-4

MDL: MFCD00012742

TNP: TNP00487



LogP: 3.18

LogS: -3.97

Acceptors: 4

Donors: 5

Rotation Bonds: 6

Chiral Centers: 1

N+O: 5

LIPINSKY: 4

Info: Alkaloid derivative of dopamine and biosynthetic precursor of morphine

IUPAC: 1-[(3,4-dihydroxyphenyl)methyl]-1,2,3,4-tetrahydroisoquinoline-6,7-diol, bromide

Smiles: Br.c1(ccc(c(c1)O)O)CC1c2c(CCN1)cc(c(c2)O)O