



Formula: C₃₂H₄₅BrN₂O₉

MW: 681.62

MDL:

TNP: TNP00013



LogP: 2.98

LogS: -3.64

Acceptors: 9

Donors: 3

Rotation Bonds: 4

Chiral Centers: 12

N+O: 11

LIPINSKY: 3

IUPAC: {2-(((1S,3S,4S,6S,8S,9S,13S,16S,5R)-11-ethyl-3,8-dihydroxy-4,6,16-trimethoxy-1 1-azahexacyclo[7.7.2.1<2,5>.0<1,10>.0<3,8>.0<13,17>]nonadec-13-yl)oxycarbonyl] phenyl}amino acetate, bromide

Smiles:

Br.N(OC(C)=O)c1ccccc1C(O[C@]12CC[C@H](OC)[C@@]34C1CC([C@H]3[N@](C2)CC)[C@
@]1(O)C[C@@H]([C@@H]2[C@@H]([C]1(O)C4C2)OC)OC)=O