

Ergotamine, dihydro, methanesulfonate (salt)

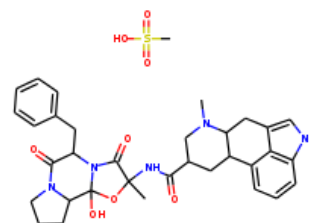
InChI: InChI=1S/C33H37N5O5.CH4O3S/c1-32(35-29(39)21-15-23-22-10-6-11-24-28(22)20(17-34-24)16-25(23)36(2)18-21)31(41)38-26(14-19-8-4-3-5-9-19)30(40)37-13-7-12-27(37)33(38,42)43-32;1-5(2,3)4/h3-6,8-11,17,21,23,25-27,34,42H,7,12-16,18H2,1-2H3,(H,35,39);1H3,(H,2,3,4)

InChI Key: ADYPXRFPBQGGAH-UHFFFAOYSA-N

Formula: C34H41N5O8S

SMILES: CN1CC(C(=O)NC2(C)OC3(O)C4CCCN4C(=O)C(Cc4ccccc4)N3C2=O)CC2c3cccc4[nH]cc(c43)CC21.CS(=O)(=O)O

Molecular Weight: 679.78



Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C33H37N5O5.CH4O3S/c1-32\(35-29\(39\)21-15-23-22-10-6-11-24-28\(22\)20\(17-34-24\)16-25\(23\)36\(2\)18-21\)31\(41\)38-26\(14-19-8-4-3-5-9-19\)30\(40\)37-13-7-12-27\(37\)33\(38,42\)43-32;1-5\(2,3\)4/h3-6,8-11,17,21,23,25-27,34,42H,7,12-16,18H2,1-2H3,\(H,35,39\);1H3,\(H,2,3,4\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C33H37N5O5.CH4O3S/c1-32(35-29(39)21-15-23-22-10-6-11-24-28(22)20(17-34-24)16-25(23)36(2)18-21)31(41)38-26(14-19-8-4-3-5-9-19)30(40)37-13-7-12-27(37)33(38,42)43-32;1-5(2,3)4/h3-6,8-11,17,21,23,25-27,34,42H,7,12-16,18H2,1-2H3,(H,35,39);1H3,(H,2,3,4))

Legend

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