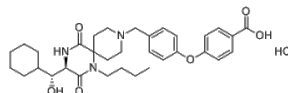


产品名称 : Aplaviroc hydrochloride

同义词 : AK-602 | GW 873140 | ONO-4128 | GSK-873140

产品货号 : M14551

CAS Number : 461023-63-2



分子式 : C₃₃H₄₄ClN₃O₆

分子量 : 614.18

化学全名 : 4-[4-[[[(3R)-1-butyl-3-[(R)-cyclohexyl(hydroxy)methyl]-2,5-dioxo-1,4,9-triazaspiro[5.5]undecan-9-yl]methyl]phenoxy]benzoic acid hydrochloride

产品描述 : Aplaviroc (GSK-873140;GW 873140;AK-602;ONO-4128) is a potent, noncompetitive, allosteric antagonist of the CCR5 receptor with pK_b of 8.6; blocks the calcium response effects of CCR5 activation by CCL5, and potently blocks in vitro the infection of R5-tropic HIV-1 (R5-HIV-1) at subnanomolar IC₅₀. HIV Infection Phase 3 Discontinued.

通路 : GPCR/G Protein

靶点 : Chemokine Receptor

受体 : Chemokine Receptor

溶解度 : In Vitro: ?DMSO : 200 mg/mL (325.64 mM)

SMILES : CCCCN1C(=O)C(NC(=O)C12CCN(CC2)CC3=CC=C(C(C=3)OC4=CC=C(C(C=C4)C(=O)O)C(C5CCCCC5)O)O)Cl

存储条件 : (-20℃)

稳定性 : ≥ 2 years

参考文献 :

1. Watson C, et al. Mol Pharmacol. 2005 Apr;67(4):1268-82. 2. Lalezari J, et al. AIDS. 2005 Sep 23;19(14):1443-8. 3. Adkison KK, et al. Antimicrob Agents Chemother. 2005 Jul;49(7):2802-6. 4. Nakata H, et al. Antimicrob Agents Chemother. 2008 Jun;52(6):2111-9.

仅限科学研究使用，不得用于人体。