



ClH

Formula: C₁₄H₂₅ClN₂O₇

MW: 368.81

Salt: 2HCl

CAS: 22189-32-8

TNP NUMBER: TNP00296

MDL NUMBER: MFCD06662299

IUPAC: (8S,11S,13S,14S,1R,3R,6R,10R,12R)-12,14-bis(methylamino)-3,11,13-trihydroxy-6-methyl-2,7,9-trioxatricyclo[8.4.0.0]tetradecan-4-one, chloride

Smiles:

N(C)[C@@H]1[C@@H]2([C@H](O[C@H]3([C@](O2)(O)C(=O)C[C@H](O3)C))([C@H]([C@@H]([C@@H]1O)NC)O)).Cl

THERAPEUTIC CATEGORY: Antibacterial

VET THERAP CATEGORY: Antibacterial

SOURCE: Antibiotic isolated from fermentation broth of Streptomices Spectabilis

ACCEPTORS: 7

DONORS: 5

ROTATION BONDS: 0

N+O: 9

Chiral Centers: 9

LogP: -4.73

LogS: -1.77

LIPINSKI: 4

