



Formula: C<sub>16</sub>H<sub>20</sub>N<sub>6</sub>O<sub>2</sub>

MW: 328.37

MDL: MFCD02063158

TNP:



LogP: 1.36

LogS: -3.4

Acceptors: 2

Donors: 1

Rotation Bonds: 4

Chiral Centers: 3

N+O: 8

LIPINSKY: 4

IUPAC: 11-((3E)-2-hydroxy-4-(1,2,4-triazol-4-yl)-4-azabut-3-enyl)-7,11-diazatricyclo[7.3.1.0<2,7>]trideca-2,4-dien-6-one

Smiles: c12n(c(ccc2)=O)CC2CN(CC1C2)CC(C=Nn1cnc1)O