



Formula: C<sub>25</sub>H<sub>27</sub>N<sub>5</sub>O<sub>3</sub>

MW: 445.52

MDL: MFCD02063152

TNP:



LogP: 2.36

LogS: -3.81

Acceptors: 3

Donors: 0

Rotation Bonds: 3

Chiral Centers: 2

N+O: 8

LIPINSKY: 4

IUPAC: 11-[(3E)-4-(2,3-dimethyl-5-oxo-1-phenyl(3-pyrazolin-4-yl))-2-oxo-4-azabut-3-en yl]-7,11-diazatricyclo[7.3.1.0<2,7>]trideca-2,4-dien-6-one

Smiles: c1(c(n(c2ccccc2)n(c1C)C)=O)/N=CC(CN1CC2c3ccccc(n3CC(C1)C2)=O)=O