



Formula: C<sub>23</sub>H<sub>28</sub>N<sub>4</sub>O<sub>2</sub>

MW: 392.5

CAS: 3151183-21-2

MDL NUMBER: MFCD02051977

IUPAC: N-[(1Z)-2-(2-hydroxy-3-prop-2-enylphenyl)-1-azavinyl]-2-[4-benzylpiperazinyl]acetamide

Smiles: C(NN=C/c1c(c(CC=C)ccc1)O)(CN1CCN(CC1)Cc1cccc1)=O

REFERENCE: 1 Putt, K.S., Chen, G.W., Pearson, J.M., et al. Small-molecule activation of procaspase-3 to caspase-3 as a personalized anticancer strategy. *Nature Chemical Biology* 2(10) 543-550 (2006).

ACCEPTORS: 2

DONORS: 2

ROTATION BONDS: 6

N+O: 6

Chiral Centers: 0

LogP: 3.12

LogS: -4.73

LIPINSKI: 4

