



Formula: C₅₂H₆₂N₄O₈

MW: 871.09

MDL:

TNP:



LogP: 1.31

LogS: -3.21

Acceptors: 8

Donors: 8

Rotation Bonds: 13

Chiral Centers: 0

N+O: 12

LIPINSKY: 2

IUPAC: N-[(1E)-2-(7-{8-[(1E)-2-(adamantanylethylamino)-2-azavinyl]-1,6,7-trihydroxy-3-methyl-5-(methylethyl)(2-naphthyl)}-2,3,8-trihydroxy-6-methyl-4-(methylethyl)naphthyl)-1-azavinyl]adamantanylethylamide

Smiles:

c1(c2c(c3c(/C=NNC(=O)C45CC6CC(CC(C6)C5)C4)c(O)c(c(c3cc2C)C(C)C)O)O)c(c2c(/C=NNC(=O)C34CC5CC(CC(C5)C4)C3)c(O)c(c(c2cc1C)C(C)C)O)O