



Formula: C₄₈H₅₂N₂O₈S₂

MW: 849.08



LogP: -2.32

LogS: -1.92

Acceptors: 8

Donors: 6

Rotation Bonds: 17

Chiral Centers: 0

N+O: 10

LIPINSKY: 2

IUPAC: 8-[(1E)-4-(4-methylthiophenoxy)-2-azabut-1-enyl]-2-{8-[(1E)-4-(4-methylthiophe noxy)-2-azabut-1-enyl]-1,6,7-trihydroxy-3-methyl-5-(methylethyl)(2-naphthyl)}-3-methyl-5-(methylethyl)naphthalene-1,6,7-triol

Smiles:

c1(c2c(c3c(/C=NCCOc4ccc(cc4)SC)c(O)c(c(c3cc2C)C(C)C)O)O)c(c2c(/C=NCCOc3ccc(cc3)SC)c(O)c(c(c2cc1C)C(C)C)O)O