



Formula: C<sub>22</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub>

MW: 406.53

MDL NUMBER: MFCD01416873

IUPAC: 4-[(3-cyano-4-(2-thienyl)-2-5,6,7,8-tetrahydroquinolythio)methyl]benzoic acid

Smiles: c1(c(c(nc2c1CCCC2)SCc1ccc(cc1)C(O)=O)C#N)c1cccs1

ACCEPTORS: 2

DONORS: 1

ROTATION BONDS: 4

N+O: 4

Chiral Centers: 0

LogP: 6.44

LogS: -5.65

LIPINSKI: 3

