



Formula: C₁₅H₁₉N₃OS

MW: 289.4

MDL: MFCD02063223

TNP:



LogP: 16.8

LogS: -10.61

Acceptors: 1

Donors: 0

Rotation Bonds: 4

Chiral Centers: 2

N+O: 4

LIPINSKY: 3

IUPAC: 3-(6-oxo-7,11-diazatricyclo[7.3.1.0<2,7>]trideca-2,4-dien-11-yl)propanisothiocyanate

Smiles: C(N=C=S)CCN1CC2Cn3c(C(C1)C2)cccc3=O