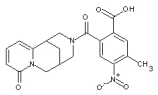

Formula: C20H19N3O6

MW: 397.39

MDL: MFCD01789905

TNP:

LogP: 1.99

LogS: -3.98

Acceptors: 6

Donors: 1

Rotation Bonds: 3

Chiral Centers: 2

N+O: 9

LIPINSKY: 4

IUPAC: 5-methyl-4-nitro-2-[(6-oxo-7,11-diazatricyclo[7.3.1.0<2,7>]trideca-2,4-dien-11 -yl)carbonyl]benzoic acid

Smiles: Cc1c([N+]([O-])=O)cc(C(N2CC3Cn4c(C(C2)C3)cccc4=O)=O)c(c1)C(=O)O