



Formula: C₃₄H₄₁N₅O₈S

MW: 679.79

CAS: 6190-39-2

TNP NUMBER: TNP00147

MDL NUMBER: MFCD05618219

Smiles:

CN1[C@@H]2(Cc3c4c(cccc4[nH]c3)[C@H]2C[C@H](C(N[C@@]2(O[C]3(N(C2=O)[C@H](C(N2[C@H]3(CCC2))=O)Cc2ccccc2)O)C)=O)(C1)).CS(O)(=O)=O

THERAPEUTIC CATEGORY: Antimigraine

REFERENCE: Merck, 13, 3196

SOURCE: Ergot Alkaloids. Preparation from ergotamine

ACCEPTORS: 8

DONORS: 4

ROTATION BONDS: 1

N+O: 13

Chiral Centers: 7

LogP: 3.71

LogS: -5.99

LIPINSKI: 3

