



Formula: C₂₂H₂₈O₁₃

MW: 500.46

CAS: 97938-28-8

MDL: MFCD09699779

TNP: TNP00627



LogP: 0.87

LogS: -3.07

Acceptors: 13

Donors: 6

Rotation Bonds: 12

Chiral Centers: 10

N+O: 13

LIPINSKY: 2

IUPAC: 6-methoxy-7-{3,4,5-trihydroxy-6-[(3,4,5-trihydroxy-6-methyl(2H-3,4,5,6-tetrahydropyran-2-yl)oxy)methyl](2H-3,4,5,6-tetrahydropyran-2-yl)oxy}chromen-2-one

Smiles: O(C1C(C(O)C(O)C(C)O1)O)CC1OC(C(C(C1O)O)O)Oc1cc2oc(ccc2cc1OC)=O

SOURCE: A coumarin glycoside from *Haplophyllum perforatum*