



Formula: C₂₈H₃₈O₁₇

MW: 646.6

MDL: MFCD09699679

TNP: TNP00629



LogP: 2.41

LogS: -3.79

Acceptors: 17

Donors: 8

Rotation Bonds: 16

Chiral Centers: 15

N+O: 17

LIPINSKY: 1

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

Smiles:

O(C1OC(C(C(C1O)O)O)C)CC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)C)Oc1cc2c(cc1OC)ccc(=O)o2

SOURCE: Coumarine