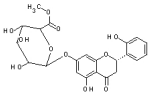

Formula: C22H22O11

MW: 462.41

MDL:

TNP:

LogP: 2.28

LogS: -3.59

Acceptors: 11

Donors: 5

Rotation Bonds: 9

Chiral Centers: 6

N+O: 11

LIPINSKY: 3

IUPAC: methyl 6-[(2S)-5-hydroxy-2-(2-hydroxyphenyl)-4-oxochroman-7-yloxy]-3,4,5-trihy droxy-2H-3,4,5,6-tetrahydropyran-2-carboxylate

Smiles: O1C(C(O)C(O)C(O)C1C(OC)=O)Oc1cc2c(C(C[C@H](O2)c2ccccc2O)=O)c(O)c1

SOURCE: Flavanone derivative