



Formula: C₂₉H₃₄O₁₆

MW: 638.58

MDL: MFCD09699809

TNP:

SCUTELLAREIN 7-O-RUTINOSIDE



LogP: 6.14

LogS: -5.59

Acceptors: 16

Donors: 8

Rotation Bonds: 16

Chiral Centers: 10

N+O: 16

LIPINSKY: 0

IUPAC: 5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-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-4-one

Smiles:

O1C(OCC2OC(C(C2O)O)O)Oc2c(c(c3c(c2)oc(c2ccc(c(c2)OC)O)cc3=O)O)OC)C(C(C(C1C)O)O)O

REFERENCE: M. P. Yuldashev1, V. M. Malikov1 Contact Information and