



Formula: C<sub>35</sub>H<sub>34</sub>O<sub>18</sub>

MW: 742.64

MDL: MFCD05725882

TNP:

CICHORIN; DEMETHYLSCOPOLIN; ESCULETIN 7-O-GLUCOSIDE



LogP: 7.47

LogS: -6.1

Acceptors: 18

Donors: 0

Rotation Bonds: 18

Chiral Centers: 5

N+O: 18

LIPINSKY: 1

IUPAC: 2-acetyloxy-4-{5-acetyloxy-4-oxo-7-[3,4,5-triacetyloxy-6-(acetyloxymethyl)(2H-3,4,5,6-tetrahydropyran-2-yloxy)]chromen-3-yl}phenyl acetate

Smiles:

c1(cc(c2c(=O)c(c3cc(c(cc3)OC(C)=O)OC(=O)C)coc2c1)OC(=O)C)OC1OC(C(C(C1OC(C)=O)OC(=O)C)OC(=O)C)COC(=O)C

SOURCE: Isoflavone for example from: *Maackia amurensis* Rupr. et. Maxim.

Specification: DEMETHYLSCOPOLIN

DEMETHYLSCOPOLIN Usage And Synthesis DEMETHYLSCOPOLIN