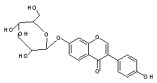

Formula: C21H20O9

MW: 416.38

CAS: 552-66-9

MDL: MFCD01871344

TNP:

4h-1-benzopyran-4-one,7-(beta-d-glucopyranosyloxy)-3-(4-hydroxyphenyl)-5-hydro;
7-(beta-d-glucopyranosyloxy)-3-(4-hydroxyphenyl)-5-hydroxy-4h-1-benzopyran-4;
7-(beta-d-glucopyranosyloxy)-3-(4-hydroxyphenyl)-5-hydroxy-4h-1-benzopyran-4-on;
7,4-dihydroxyisofla

LogP: 2.77

LogS: -4.1

Acceptors: 9

Donors: 5

Rotation Bonds: 8

Chiral Centers: 5

N+O: 9

LIPINSKY: 4

IUPAC: 3-(4-hydroxyphenyl)-7-[3,4,5-trihydroxy-6-(hydroxymethyl)(2H-3,4,5,6-tetrahydr
opyran-2-yloxy)]chromen-4-one

Smiles: c1(c2c(c3ccc(OC4OC(C(C(C4O)O)O)CO)cc3oc2)=O)ccc(O)cc1

Specification: pharmacetical; The group of Daidzin; Intermediates & Fine Chemicals; Pharmaceuticals Daidzin Chemical Properties:

mp 234-236C alpha -24