



Formula: C<sub>21</sub>H<sub>22</sub>O<sub>9</sub>

MW: 418.4

MDL: MFCD09699810

TNP:



LogP: -1.2

LogS: -2.12

Acceptors: 9

Donors: 5

Rotation Bonds: 8

Chiral Centers: 6

N+O: 9

LIPINSKY: 4

IUPAC: 2-(4-hydroxyphenyl)-7-[3,4,5-trihydroxy-6-(hydroxymethyl)(2H-3,4,5,6-tetrahydropyran-2-yl)oxy]chroman-4-one

Smiles: OCC1OC(C(C(C1O)O)O)Oc1ccc2C(=O)CC(c3ccc(O)cc3)Oc2c1

SOURCE: A flavone glycoside isolated from licorice