



Formula: C₂₇H₃₀O₁₄

MW: 578.53

CAS: 64820-99-1

MDL:

TNP:



LogP: 3.56

LogS: -4.53

Acceptors: 14

Donors: 9

Rotation Bonds: 4

Chiral Centers: 10

N+O: 14

LIPINSKY: 1

Info: C-glycoside Flavonoid, isolated from many plants

IUPAC: 8-[(2S,4S,5S,3R,6R)-3-((2S,6S,3R,4R,5R)-3,4,5-trihydroxy-6-methyl(2H-3,4,5,6-tetrahydropyran-2-yl)oxy))-4,5-dihydroxy-6-(hydroxymethyl)(2H-3,4,5,6-tetrahydropyran-2-yl)]-5,7-dihydroxy-2-(4-hydroxyphenyl)chromen-4-one

Smiles:

c12[c@@](C3[C@@H]([C@@H](O)[C@@H]([C@H](O3)CO)O)O[C@H]3[C@@H]([C@@H]([C@@H](O)[C@@H](O3)CO)O)O)c(cc(c1c(cc(o2)c1ccc(O)cc1)=O)O)O

