



Formula: C₂₁H₂₀O₉

MW: 416.38

CAS: 3681-99-0

TNP NUMBER: TNP00649

MDL NUMBER: MFCD03854203

IUPAC: 7-hydroxy-3-(4-hydroxyphenyl)-8-[3,4,5-trihydroxy-6-(hydroxymethyl)(2H-3,4,5,6-tetrahydropyran-2-yl)]chromen-4-one

Smiles: c12c(C3OC(CO)C(C(C3O)O)O)c(O)ccc1c(=O)c(co2)c1ccc(cc1)O

Puerarin is the most concentrated isoflavone found in kudzu

THERAPEUTIC CATEGORY: Puerarin has potential antioxidant activity and impairs CYP catalyzed drug metabolism [1]. It's metabolite calycosin has cytotoxic activity [2].

ACCEPTORS: 9

DONORS: 6

ROTATION BONDS: 8

N+O: 9

Chiral Centers: 5

LogP: -1.12

LogS: -2.96

LIPINSKI: 3

Synonyms:

DAIDZEIN-8-C-GLUCOSIDE;8-GLUCOSYLD Aidzein;7-HYDROXY-3-[4-HYDROXYPHENYL]-1-BENZOPYRAN-4-ONE

8-[BETA-D-GLUCOPYRANOSIDE;7,4'-DIHYDROXY-8-C-GLUCOSYLISOFLAVONE;8-(beta-d-glucopyranosyl-7-hydroxy-3-(4-hydroxyphenyl)-4h-1-benzopyran-4-one;4',7-DIHYDROXY-8-C-GLUCOSYLISOFLAVONE;PUERARIN;Puerarin

CAS:3681-99-0

MF:C21H20O10

MW:432.38

EINECS:

Product Categories:Iso-Flavones;Natural Plant Extract Puerarin

Chemical Properties: mp 187-189C

CAS DataBase Reference: 3681-99-0(

CAS DataBase Reference:) F,C Risk Statements 11-34 Safety Statements 22-24/25-45-36/37/39-26-16 WGK Germany 3 RTECS UO5216000 F 10 Puerarin

Usage And Synthesis: Puerarin

