



Formula: C₁₅H₁₂O₈

MW: 320.26

Salt: 2 H₂O

MDL:

TNP: TNP00089



LogP: -3.96

LogS: -2.56

Acceptors: 8

Donors: 7

Rotation Bonds: 6

Chiral Centers: 0

N+O: 8

LIPINSKY: 3

Info: Widely available organic acid prepared by isomerization of rosin

IUPAC: 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxychromen-4-one, hydrate

Smiles: c1(c(oc2cc(O)cc(c2c1=O)O)c1cc(O)c(cc1)O)O.O