



Formula: C₂₇H₃₀O₁₆

MW: 610.53

Salt: 3H₂O

CAS: 153-18-4

TNP NUMBER: TNP00554

MDL NUMBER: MFCD09787952

IUPAC: 3-{6-[(6S,2R,3R,4R,5R)-3,4,5-trihydroxy-6-methyl(2H-3,4,5,6-tetrahydropyran-2-ylloxy)]methyl}(2S,4S,5S,3R,6R)-3,4,5-trihydroxy(2H-3,4,5,6-tetrahydropyran-2-ylloxy)}-2-(2,3-dihydroxyphenyl)-5,7-dihydroxychromen-4-one

Smiles:

C[C@@H]1O[C@H]([C@@H]([C@@H]([C@H]1O)O)O)OC[C@H]1O[C@H]([C@H](O)[C@H]([C@@H]1O)O)Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cccc(O)c1O

Found in many plants, especially in black wheat plants

THERAPEUTIC CATEGORY: Capillary protectant

ACCEPTORS: 16

DONORS: 10

ROTATION BONDS: 7

N+O: 16

Chiral Centers: 10

LogP: -4.94

LogS: -2.27

LIPINSKI: 1

Synonyms: 3,3