

Protocatechuic acid 4-O-glucoside; DTXSID301341731

Compound CID: 157010113

MF: C₁₃H₁₆O₉ MW: 316.26 g/mol

IUPAC Name: 3-hydroxy-4-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-

yl]oxybenzoic acid

SMILES: C1=CC(=C(C=C1C(=O)O)O)OC2C(C(C(C(O2)CO)O)O)O

InChlKey: HFFREILXLCWCQH-UHFFFAOYSA-N

InChl: InChl=1S/C13H16O9/c14-4-8-9(16)10(17)11(18)13(22-8)21-7-2-1-

5(12(19)20)3-6(7)15/h1-3,8-11,13-18H,4H2,(H,19,20)

Create Date: 2021-11-15

Summary

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5-fluoro-protocatechuic acid; SCHEMBL9787632

Compound CID: 15173704

MF: C₇H₅FO₄ MW: 172.11 g/mol

IUPAC Name: 3-fluoro-4,5-dihydroxybenzoic acid

SMILES: C1=C(C=C(C(=C1O)O)F)C(=O)O

InChlKey: RTYDIWLGIZQTKB-UHFFFAOYSA-N

InChl: InChl=1S/C7H5FO4/c8-4-1-3(7(11)12)2-5(9)6(4)10/h1-2,9-10H,

(H,11,12)

Create Date: 2007-02-09

Summary

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