



Formula: C₁₂H₁₀O₅

MW: 234.21

CAS: 5852-10-8

MDL: MFCD00467589

TNP: TNP00568

7-HYDROXY-4-METHYLCOUMARIN-3-ACETIC ACID;
(7-HYDROXY-4-METHYL-2-OXO-2H-CHROMEN-3-YL)-ACETIC ACID;
7-HYDROXY-4-METHYL-3-COUMARINYLACETIC ACID;
7-HYDROXY-4-METHYL-CUMARONE-3-YL ACETIC ACID;
4-METHYLBELLIFERONE-3-ACETIC ACID;
7-HYDROXY-4-METHYL-3-COUMARINYLACET



LogP: 2.17

LogS: -4.43

Acceptors: 5

Donors: 2

Rotation Bonds: 4

Chiral Centers: 0

N+O: 5

LIPINSKY: 4

IUPAC: 2-(7-hydroxy-4-methyl-2-oxochromen-3-yl)acetic acid

Smiles: c1(c(oc2c(c1C)ccc(O)c2)=O)CC(=O)O

Specification: 7-HYDROXY-4-METHYL-3-COUMARINYLACETIC ACID Chemical Properties:

mp 263-267 C solubility DMF: soluble Safety Information Hazard Codes Xi Risk Statements

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7-HYDROXY-4-METHYL-3-COUMARINYLACETIC ACID Usage And Synthesis

7-HYDROXY-4-METHYL-3-COUMARINYLACETIC ACID Raw materials Etanol-->Sodium

hydroxide-->Hydrochloric acid-->Diethyl ether-->Sulfuric acid -->Sodium-->Magnesium

sulfate-->Triethylamine-->Acetone-->Ethyl acetoacetate-->Resorcine-->Bromoacetic

acid-->Cupric bromide