



Formula: C<sub>12</sub>H<sub>10</sub>O<sub>5</sub>

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  
36/37/38 Safety Statements 26-36 WGK Germany 3 F 8  
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