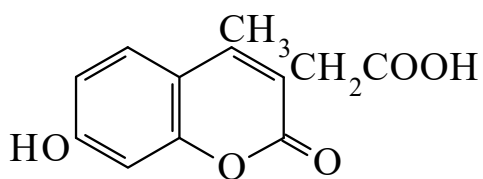




>>Entry Name: 7-Hydroxy-4-methyl-2-oxo-2*H*-1-benzopyran-3-acetic acid, 9CI
Synonym(s): 7-Hydroxy-4-methylcoumarin-3-acetic acid. 4-Methylumbelliferone-3-acetic acid



CAS Registry Number: 5852-10-8

Molecular Formula: C₁₂H₁₀O₅
Molecular Weight: 234.208
Accurate Mass: 234.052825
Percentage Composition: C 61.54%; H 4.30%; O 34.16%
Use/Importance: Fluorescent label
Physical Description: Needles (EtOH aq.)
Melting Point: Mp 268°

>>Derivative: Et ester

Molecular Formula: C₁₄H₁₄O₅
Molecular Weight: 262.262
Accurate Mass: 262.084125
Percentage Composition: C 64.12%; H 5.38%; O 30.50%
Physical Description: Needles (Me₂CO/EtOH)
Melting Point: Mp 163°

>>Derivative: Ac

Molecular Formula: C₁₄H₁₂O₆
Molecular Weight: 276.245
Accurate Mass: 276.06339
Percentage Composition: C 60.87%; H 4.38%; O 34.75%
Melting Point: Mp 199-200°

>>Derivative: Ac, Et ester

Molecular Formula: C₁₆H₁₆O₆
Molecular Weight: 304.299
Accurate Mass: 304.09469
Percentage Composition: C 63.15%; H 5.30%; O 31.55%
Physical Description: Fine leaflets (EtOH aq.)
Melting Point: Mp 98°

>>Derivative: Benzoyl

Molecular Formula: C₁₉H₁₄O₆
Molecular Weight: 338.316
Accurate Mass: 338.07904
Percentage Composition: C 67.45%; H 4.17%; O 28.37%
Melting Point: Mp 190-191°

>>Derivative: Benzoyl, Et ester

Molecular Formula: C₂₁H₁₈O₆
Molecular Weight: 366.37
Accurate Mass: 366.11034
Percentage Composition: C 68.85%; H 4.95%; O 26.20%
Melting Point: Mp 138°