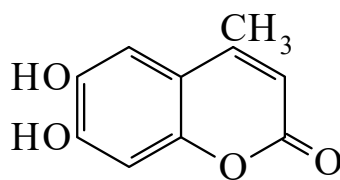




>>Entry Name: 6,7-Dihydroxy-4-methyl-2*H*-1-benzopyran-2-one, 9Cl

ENTRY UNDER REVIEW

Synonym(s): 6,7-Dihydroxy-4-methylcoumarin. 4-Methylaesculetin



CAS Registry Number: 529-84-0

Related CAS Registry Numbers(s): 1040-23-9

Molecular Formula: C₁₀H₈O₄

Molecular Weight: 192.171

Accurate Mass: 192.04226

Percentage Composition: C 62.50%; H 4.20%; O 33.30%

Use/Importance: Used as 1% soln. in EtOH as a redox fluorescent indicator. Used as 1mM soln. in EtOH for photometric detn. of Mo(VI), Nb(V), Ti(IV)

Physical Description: Yellow cryst. (EtOH aq.)

Melting Point: Mp 272-274°

pKa Value: pK_{a1} 7.44; pK_{a2} 8.12

Aldrich: 11990-3

Sigma: D6275

>>Derivative: Bis(hydrogen sulfate)

Synonym(s): Sulmarin, INN, USAN. 4-Methyl-6,7-bis(sulfooxy)-2*H*-1-benzopyran-2-one, 9Cl. MG 143. Idro P₂

CAS Registry Number: 29334-07-4

Molecular Formula: C₁₀H₈O₁₀S₂

Molecular Weight: 352.299

Accurate Mass: 351.95589

Percentage Composition: C 34.09%; H 2.29%; O 45.41%; S 18.20%

Use/Importance: Haemostatic drug, used as di-Na salt

>>Derivative: Di-Ac

CAS Registry Number: 55939-28-1

Molecular Formula: C₁₄H₁₂O₆

Molecular Weight: 276.245

Accurate Mass: 276.06339

Percentage Composition: C 60.87%; H 4.38%; O 34.75%

Physical Description: Cryst. (C₆H₆)

Aldrich: 31744-6

Sigma: D3912

>>Derivative: Di-Me ether

Synonym(s): 6,7-Dimethoxy-4-methyl-2*H*-1-benzopyran-2-one

CAS Registry Number: 4281-40-7

Molecular Formula: C₁₂H₁₂O₄

Molecular Weight: 220.224

Accurate Mass: 220.07356

Percentage Composition: C 65.45%; H 5.49%; O 29.06%

Melting Point: Mp 136-139°

Aldrich: 31640-7

Sigma: D4037