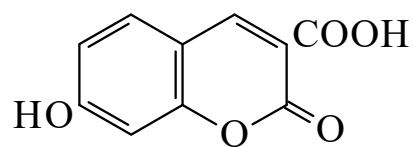




>>Entry Name: 7-Hydroxy-2-oxo-2*H*-1-benzopyran-3-carboxylic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 7-Hydroxycoumarin-3-carboxylic acid. Umbelliferone-3-carboxylic acid



CAS Registry Number: 779-27-1

Molecular Formula: C₁₀H₆O₅

Molecular Weight: 206.154

Accurate Mass: 206.021525

Percentage Composition: C 58.26%; H 2.93%; O 38.80%

Use/Importance: Used for fluorimetric detn. of amines

Physical Description: Cryst.

Melting Point: Mp 271 dec.°

Sigma: H8028

>>Derivative: Me ester

CAS Registry Number: 86788-49-0

Molecular Formula: C₁₁H₈O₅

Molecular Weight: 220.181

Accurate Mass: 220.037175

Percentage Composition: C 60.01%; H 3.66%; O 36.33%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 236-237°

>>Derivative: Et ester

CAS Registry Number: 6093-71-6

Molecular Formula: C₁₂H₁₀O₅

Molecular Weight: 234.208

Accurate Mass: 234.052825

Percentage Composition: C 61.54%; H 4.30%; O 34.16%

Physical Description: Cryst.

Melting Point: Mp 171°

Sigma: H8153

>>Derivative: Nitrile

Synonym(s): 7-Hydroxy-3-cyanocoumarin

CAS Registry Number: 19088-73-4

Molecular Formula: C₁₀H₅NO₃

Molecular Weight: 187.154

Accurate Mass: 187.026944

Percentage Composition: C 64.18%; H 2.69%; N 7.48%; O 25.65%

Physical Description: Yellow rectangular plates (EtOH)

Melting Point: Mp 270-272° (262°)

>>Derivative: Ac

CAS Registry Number: 81017-23-4

Molecular Formula: C₁₂H₈O₆

Molecular Weight: 248.192

Accurate Mass: 248.03209

Percentage Composition: C 58.07%; H 3.25%; O 38.68%

Physical Description: Cryst. (AcOH)

Melting Point: Mp 208°