



>>Entry Name: 2-Oxo-2H-1-benzopyran-6-carboxylic acid, 9CI

Synonym(s): Coumarin-6-carboxylic acid

CAS Registry Number: 7734-80-7

Molecular Formula: C₁₀H₆O₄

Molecular Weight: 190.155

Accurate Mass: 190.02661

Percentage Composition: C 63.16%; H 3.18%; O 33.66%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 268°

Other Data: Blue fluor. in alkaline sol.

>>Derivative: Me ester

Molecular Formula: C₁₁H₈O₄

Molecular Weight: 204.182

Accurate Mass: 204.04226

Percentage Composition: C 64.71%; H 3.95%; O 31.34%

Physical Description: Needles (petrol/C₆H₆)

Melting Point: Mp 174°

>>Derivative: Et ester

Molecular Formula: C₁₂H₁₀O₄

Molecular Weight: 218.209

Accurate Mass: 218.05791

Percentage Composition: C 66.05%; H 4.62%; O 29.33%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 130°

>>Derivative: Amide

CAS Registry Number: 7734-81-8

Molecular Formula: C₁₀H₇NO₃

Molecular Weight: 189.17

Accurate Mass: 189.042594

Percentage Composition: C 63.49%; H 3.73%; N 7.40%; O 25.37%

Physical Description: Prisms (H₂O)

Melting Point: Mp 203°. Mp 251-252°

>>Derivative: Anilide

Molecular Formula: C₁₆H₁₁NO₃

Molecular Weight: 265.268

Accurate Mass: 265.073894

Percentage Composition: C 72.45%; H 4.18%; N 5.28%; O 18.09%

Physical Description: Cryst. (AcOH)

Melting Point: Mp 194°

>>Derivative: Nitrile

Synonym(s): 6-Cyanocoumarin

CAS Registry Number: 50396-61-7

Molecular Formula: C₁₀H₅NO₂

Molecular Weight: 171.155

Accurate Mass: 171.032029

Percentage Composition: C 70.18%; H 2.94%; N 8.18%; O 18.70%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 224-226°. Mp 220°

References:

- Stoermer, R. *et al.*, *Ber.*, 1904, **37**, 192, (*synth, deriv*)
Dey, B.B. *et al.*, *J.C.S.*, 1923, **123**, 3384, (*synth, derivs*)
Hershfield, R. *et al.*, *J.A.C.S.*, 1973, **95**, 7359, (*derivs*)
Gottlieb, H.E. *et al.*, *J.C.S. Perkin 2*, 1979, 435, (*cmr*)
Morphy, J.R. *et al.*, *J.C.S. Perkin 2*, 1990, 573, (*nitrile*)