



>>Entry Name: 7-Hydroxy-4-oxo-4*H*-1-benzopyran-2-carboxylic acid, 9CI
Synonym(s): 7-Hydroxychromone-2-carboxylic acid

CAS Registry Number: 30113-83-8

Molecular Formula: C₁₀H₆O₅
Molecular Weight: 206.154
Accurate Mass: 206.021525
Percentage Composition: C 58.26%; H 2.93%; O 38.80%
Physical Description: Cryst. (EtOH aq.)
Melting Point: Mp 307-308°

>>Derivative: Et ester

CAS Registry Number: 23866-72-0
Molecular Formula: C₁₂H₁₀O₅
Molecular Weight: 234.208
Accurate Mass: 234.052825
Percentage Composition: C 61.54%; H 4.30%; O 34.16%
Physical Description: Yellow needles (EtOH)
Melting Point: Mp 223-224°

>>Derivative: Amide

CAS Registry Number: 36769-91-2
Molecular Formula: C₁₀H₇NO₄
Molecular Weight: 205.17
Accurate Mass: 205.037509
Percentage Composition: C 58.54%; H 3.44%; N 6.83%; O 31.19%
Physical Description: Yellow solid
Melting Point: Mp 270-271°

>>Derivative: Nitrile

Synonym(s): 2-Cyano-7-hydroxy-4*H*-1-benzopyran-4-one

CAS Registry Number: 36764-24-6
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: Cryst. (MeOH)
Melting Point: Mp 251-252°

>>Derivative: Me ether

Synonym(s): 7-Methoxy-4-oxo-4*H*-1-benzopyran-2-carboxylic acid

Molecular Formula: C₁₁H₈O₅
Molecular Weight: 220.181
Accurate Mass: 220.037175
Percentage Composition: C 60.01%; H 3.66%; O 36.33%
Melting Point: Mp 274-276 dec.° (265°)

References:

- Barker, G. *et al.*, *J.C.S.(C)*, 1970, 2230, (*synth*)
Ellis, G.P. *et al.*, *J.C.S. Perkin I*, 1981, 2557, (*Et ester, cmr*)
Manchand, P.S. *et al.*, *Tetrahedron*, 1992, **48**, 9391, (*Et ester, synth, ir, pms*)
Stoermer, M.J. *et al.*, *Aust. J. Chem.*, 1995, **48**, 677, (*synth, pmr, cmr*)
Zhang, M.-Q. *et al.*, *J. Med. Chem.*, 1995, **38**, 2472, (*nitrile, amide, synth, pmr*)