



>>Entry Name: 4-Oxo-4H-1-benzopyran-3-carboxylic acid, 9Cl, 8Cl

Synonym(s): Chromone-3-carboxylic acid

CAS Registry Number: 39079-62-4

Molecular Formula: C₁₀H₆O₄

Molecular Weight: 190.155

Accurate Mass: 190.02661

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

Use/Importance: Intermed. for synth. of many pharmaceuticals

Physical Description: Cryst. (EtOH)

Melting Point: Mp 203-204°

>>Derivative: Me ester

CAS Registry Number: 93562-17-5

Molecular Formula: C₁₁H₈O₄

Molecular Weight: 204.182

Accurate Mass: 204.04226

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

Physical Description: Cryst. (EtOAc/petrol)

Melting Point: Mp 93-94°

>>Derivative: Chloride

CAS Registry Number: 39079-63-5

Molecular Formula: C₁₀H₅ClO₃

Molecular Weight: 208.6

Accurate Mass: 207.992722

Percentage Composition: C 57.58%; H 2.42%; Cl 17.00%; O 23.01%

Melting Point: Mp 143-144°

>>Derivative: Amide

CAS Registry Number: 52817-14-8

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: Pale-yellow cryst.

Melting Point: Mp 236-238 dec.°

>>Derivative: Nitrile

Synonym(s): 4-Oxo-4H-1-benzopyran-3-carbonitrile, 9Cl

CAS Registry Number: 50743-17-4

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: Cryst. (EtOH)

Melting Point: Mp 177-178°

Aldrich: 38348-1

References:

Ellis, G.P. *et al.*, *Prog. Med. Chem.*, 1973, **9**, 65, (rev)

Nohara, A. *et al.*, *Chem. Pharm. Bull.*, 1974, **22**, 2959, (synth, ms)

Nohara, A. *et al.*, *J. Med. Chem.*, 1977, **20**, 141, (nitrile)

Ellis, G.P. *et al.*, *J. Med. Chem.*, 1978, **21**, 1120, (synth)

Cremins, P.J. *et al.*, *Tetrahedron*, 1987, **43**, 3075, (synth, deriv, ir, pmr)

Hsung, R.P. *et al.*, *J.O.C.*, 1999, **64**, 8736-8740, (nitrile, synth, pmr)