



>>Entry Name: 1-Oxo-5-indanecarboxylic acid

Synonym(s): 2,3-Dihydro-1-oxo-1*H*-indene-5-carboxylic acid, 9Cl. 5-Carboxy-1-indanone

CAS Registry Number: 3470-45-9

Molecular Formula: C₁₀H₈O₃

Molecular Weight: 176.171

Accurate Mass: 176.047345

Percentage Composition: C 68.18%; H 4.58%; O 27.25%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 272-273 dec.°

>>Derivative: Me ester

CAS Registry Number: 68634-02-6

Molecular Formula: C₁₁H₁₀O₃

Molecular Weight: 190.198

Accurate Mass: 190.062995

Percentage Composition: C 69.46%; H 5.30%; O 25.24%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 115-117°

>>Derivative: Et ester

CAS Registry Number: 150969-57-6

Molecular Formula: C₁₂H₁₂O₃

Molecular Weight: 204.225

Accurate Mass: 204.078645

Percentage Composition: C 70.58%; H 5.92%; O 23.50%

Melting Point: Mp 65°

>>Derivative: Amide

Molecular Formula: C₁₀H₉NO₂

Molecular Weight: 175.187

Accurate Mass: 175.063329

Percentage Composition: C 68.56%; H 5.18%; N 8.00%; O 18.27%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 204.5-205°

>>Derivative: Nitrile

Synonym(s): 5-Cyano-1-indanone

CAS Registry Number: 25724-79-2

Molecular Formula: C₁₀H₇NO

Molecular Weight: 157.171

Accurate Mass: 157.052764

Percentage Composition: C 76.42%; H 4.49%; N 8.91%; O 10.18%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 131.5-132°

References:

Allinger, N.L. *et al.*, *J.O.C.*, 1962, **27**, 70-76, (*synth, amide, nitrile*)

Aono, T. *et al.*, *Chem. Pharm. Bull.*, 1978, **26**, 2475-2482, (*Me ester, synth, ir, pmr*)

Takeuchi, R. *et al.*, *J.O.C.*, 1993, **58**, 5386-5392, (*Et ester, synth, ir, pmr, cmr*)

Arnold, D.R. *et al.*, *Can. J. Chem.*, 1995, **73**, 307-318, (*nitrile, synth, ir, pmr, cmr, ms*)