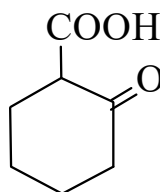




>>Entry Name: 2-Oxocyclohexanecarboxylic acid, 9Cl

Synonym(s): Cyclohexanone-2-carboxylic acid



CAS Registry Number: 18709-01-8

Molecular Formula: C₇H₁₀O₃

Molecular Weight: 142.154

Accurate Mass: 142.062995

Percentage Composition: C 59.14%; H 7.09%; O 33.76%

>>Variant: (±)-form

Molecular Formula: C₇H₁₀O₃

Molecular Weight: 142.154

Accurate Mass: 142.062995

Percentage Composition: C 59.14%; H 7.09%; O 33.76%

Physical Description: Needles (Et₂O)

Other Data: Decarboxylates at 81-2°, dec. slowly at r.t.

>>Derivative: Me ester

CAS Registry Number: 41302-34-5

Extra CAS Registry Numbers(s): 103533-31-9

Molecular Formula: C₈H₁₂O₃

Molecular Weight: 156.181

Accurate Mass: 156.078645

Percentage Composition: C 61.52%; H 7.74%; O 30.73%

Boiling Point: Bp₂ 75-85°

Refractive Index: n_D²⁵ 1.4832

>>Derivative: Et ester

CAS Registry Number: 1655-07-8

Molecular Formula: C₉H₁₄O₃

Molecular Weight: 170.208

Accurate Mass: 170.094295

Percentage Composition: C 63.51%; H 8.29%; O 28.20%

Boiling Point: Bp₁₀₀ 159-160°. Bp₁₂ 107-108°

pKa Value: pK_{a1} 10.94 (25°, 1 0.2 KCl)

Aldrich: E2000-4

Fluka: 29161

Rare Chemicals Library: S3901-3

Sigma: O0881

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 692D, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1112A, (*nmr*)

Alder, K. *et al.*, *Annalen*, 1949, **565**, 148, (*synth*)

Bierling, B. *et al.*, *J. Prakt. Chem.*, 1972, **314**, 170, (*synth*)

Shiotani, S. *et al.*, *Chem. Pharm. Bull.*, 1973, **21**, 1160-1163, (*Me ester, synth, ir, pmr*)

Christie, R.M. *et al.*, *J.C.S. Perkin I*, 1976, 880, (*synth*)

Chiba, K. *et al.*, *Chem. Lett.*, 1978, 1387, (*synth*)