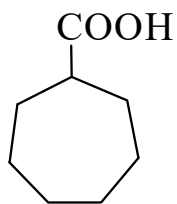




>>Entry Name: Cycloheptanecarboxylic acid, 9CI



CAS Registry Number: 1460-16-8

Molecular Formula: C₈H₁₄O₂

Molecular Weight: 142.197

Accurate Mass: 142.09938

Percentage Composition: C 67.57%; H 9.92%; O 22.50%

Physical Description: Oil

Boiling Point: Bp₇₁₁ 254-258°. Bp₈ 130-131°

Density: d₄²⁰ 1.042104

Refractive Index: n_D²⁰ 1.4753

Aldrich: C9850-0

>>Derivative: Me ester

CAS Registry Number: 60433-00-3

Molecular Formula: C₉H₁₆O₂

Molecular Weight: 156.224

Accurate Mass: 156.11503

Percentage Composition: C 69.19%; H 10.32%; O 20.48%

Boiling Point: Bp₁₁ 80°

>>Derivative: 4-Bromophenacyl ester

Melting Point: Mp 97-98°

>>Derivative: Amide

CAS Registry Number: 1459-39-8

Molecular Formula: C₈H₁₅NO

Molecular Weight: 141.213

Accurate Mass: 141.115364

Percentage Composition: C 68.04%; H 10.71%; N 9.92%; O 11.33%

Physical Description: Leaflets (PhCl)

Melting Point: Mp 195°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 835B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 538A, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 603B, (*ir*)

Reppe, W. *et al.*, *Annalen*, 1948, **560**, 1, (*synth*)

Gol'mov, V.P., *Zh. Obshch. Khim.*, 1952, **22**, 809; *CA*, **47**, 3251