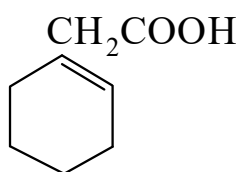




>>Entry Name: 1-Cyclohexene-1-acetic acid, 9CI



CAS Registry Number: 18294-87-6

Molecular Formula: C₈H₁₂O₂

Molecular Weight: 140.182

Accurate Mass: 140.08373

Percentage Composition: C 68.55%; H 8.63%; O 22.83%

Boiling Point: Bp₁₃ 150-155°

>>Derivative: Me ester

CAS Registry Number: 53723-52-7

Molecular Formula: C₉H₁₄O₂

Molecular Weight: 154.208

Accurate Mass: 154.09938

Percentage Composition: C 70.10%; H 9.15%; O 20.75%

Boiling Point: Bp₁₀ 84°

>>Derivative: Nitrile

Synonym(s): 1-Cyclohexene-1-acetonitrile, 9CI. 1-Cyanomethylcyclohexene

CAS Registry Number: 6975-71-9

Molecular Formula: C₈H₁₁N

Molecular Weight: 121.182

Accurate Mass: 121.089149

Percentage Composition: C 79.29%; H 9.15%; N 11.56%

Physical Description: Liq.

Boiling Point: Bp₂₅ 110-112°

Refractive Index: n_D²⁵ 1.4769

Aldrich: C10340-3

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1364C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 847A, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 805D, (*ir*)

Calvert, W. *et al.*, *J.O.C.*, 1961, **26**, 2809, (*synth*)

Org. Synth., Coll. Vol., 4, 1963, 234, (*nitrile*)

Zweifel, G. *et al.*, *J.A.C.S.*, 1977, **99**, 3184, (*synth*)

Venkateswaran, R.V. *et al.*, *Tet. Lett.*, 1979, 553, (*nitrile*)