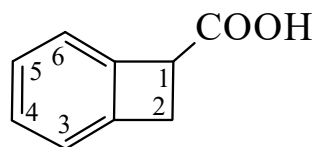




>>Entry Name: 1-Benzocyclobutenecarboxylic acid

Synonym(s): Bicyclo[4.2.0]octa-1,3,5-triene-7-carboxylic acid, 9CI



CAS Registry Number: 14381-41-0

Molecular Formula: C₉H₈O₂

Molecular Weight: 148.161

Accurate Mass: 148.05243

Percentage Composition: C 72.96%; H 5.44%; O 21.60%

General Statement: CA numbering differs

Aldrich: 32488-4

>>Variant: (±)-form

Molecular Formula: C₉H₈O₂

Molecular Weight: 148.161

Accurate Mass: 148.05243

Percentage Composition: C 72.96%; H 5.44%; O 21.60%

Physical Description: Cryst. (petrol)

Melting Point: Mp 76.5°

>>Derivative: Me ester

CAS Registry Number: 35095-07-9

Molecular Formula: C₁₀H₁₀O₂

Molecular Weight: 162.188

Accurate Mass: 162.06808

Percentage Composition: C 74.06%; H 6.21%; O 19.73%

Physical Description: Liq.

Boiling Point: Bp_{0.5} 64°

>>Derivative: Et ester

Molecular Formula: C₁₁H₁₂O₂

Molecular Weight: 176.215

Accurate Mass: 176.08373

Percentage Composition: C 74.98%; H 6.86%; O 18.16%

Physical Description: Liq.

Boiling Point: Bp_{0.7} 68°

>>Derivative: Nitrile

Synonym(s): 1-Cyanobenzocyclobutene

CAS Registry Number: 6809-91-2

Molecular Formula: C₉H₇N

Molecular Weight: 129.161

Accurate Mass: 129.057849

Percentage Composition: C 83.69%; H 5.46%; N 10.84%

Physical Description: Liq.

Boiling Point: Bp₃ 100-103°

Aldrich: 32489-2

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1001C; 1480A, (nmr)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1319C; 1399A, (ir)

Cava, M.P. *et al.*, J.A.C.S., 1958, **80**, 2255; J.O.C., 1962, **27**, 631, (synth)

Bunnett, J.F., J.O.C., 1962, **27**, 3836, (synth)

Matsuda, T., Bull. Chem. Soc. Jpn., 1966, **39**, 1342

Org. Synth., 1968, **48**, 53, (deriv)

Bubb, W.A. *et al.*, Aust. J. Chem., 1976, **29**, 1685, (pmr)