



>>Entry Name: 1,4-Cyclohexadiene, 9CI

Synonym(s): 1,4-Dihydrobenzene

CAS Registry Number: 628-41-1

Related CAS Registry Numbers(s): 12169-67-4

Extra CAS Registry Numbers(s): 29797-09-9

Structure by analogy with 1,3-Cyclohexadiene, [HDF97-Y](#)

Molecular Formula: C₆H₈

Molecular Weight: 80.129

Accurate Mass: 80.0626

Percentage Composition: C 89.94%; H 10.06%

Melting Point: Mp -49.2°

Boiling Point: Bp 86-87°

Refractive Index: n_D²⁰ 1.4725

Hazard & Toxicity: Highly flammable, fl. p. -1°

Aldrich: 12541-5

Fluka: 28908

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 62A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 46D, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 68D, (*ir*)

Stidham, H.D., *Spectrochim. Acta*, 1965, **21**, 23, (*synth, ir, Raman*)

Garbisch, E.W. *et al.*, *J.A.C.S.*, 1968, **90**, 3590, (*pmr, conformn*)

Scharf, H.D. *et al.*, *Chem. Ber.*, 1969, **102**, 2478, (*synth*)

Reimlinger, H. *et al.*, *Chem. Ber.*, 1970, **103**, 2317, (*synth*)

Dunogues, J. *Organomet. Chem.*, 1972, **43**, 127, (*synth*)

Org. Synth., 1973, **53**, 1860, (*synth*)

Marshall, J.L. *et al.*, *J.A.C.S.*, 1976, **98**, 3406, (*cmr*)

Luettker, W. *et al.*, *Chem. Ber.*, 1978, **111**, 2384, (*conformn, pmr*)

Brandsma, L. *et al.*, *Synth. Commun.*, 1990, **20**, 2165, (*synth*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, CPA750