>>**Entry Name: Heptane,** 9Cl, 8Cl
Synonym(s): Abietene (obsol.)

CAS Registry Number: 142-82-5
Related CAS Registry Numbers(s): 33838-52-7

$H_3C(CH_2)_5CH_3$

Molecular Formula: C_7H_{16}
Molecular Weight: 100.203
Accurate Mass: 100.1252
Percentage Composition: C 83.91%; H 16.09%
Biological Source: Isol. from terpentines, esp. from *Pinus* spp.
Use/Importance: Calibration standard for rating gasoline antiknock quality
Melting Point: Mp –91.61°
Boiling Point: Bp 98.3°
Density: d_4^{20} 0.684
Refractive Index: n_D^{20} 1.3877
Hazard & Toxicity: Highly flammable, fl. p. –4°, autoignition temp. 204°. Vapour irritant and narcotic in high concs. OES: long-term 400 ppm; short-term 500 ppm

Aldrich: 27051-2
Fluka: 51750
Sigma: H9629
Supelco: R42-1007

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1D, *(ir)*
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1C, *(nmr)*
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 2D, *(ir)*
Shepard, A.F. *et al.*, *J.A.C.S.*, 1931, **53**, 1948-1958, *(props)*
Orlov, N.A. *et al.*, *J. Appl. Chem. USSR (Engl. Transl.)*, 1935, **8**, 1170-1175, *(synth)*
Williams, A.L. *et al.*, *J. Pharm. Sci.*, 1962, **51**, 970-975, *(isol)*
Grant, D.M. *et al.*, *J.A.C.S.*, 1964, **86**, 2984-2990, *(cmr, pmr)*
Lavauchy, A. *et al.*, *Org. Mass Spectrom.*, 1978, **13**, 410-416, *(ms)*
Boese, R. *et al.*, *Angew. Chem., Int. Ed.*, 1999, **38**, 988-992, *(cryst struct)*
Low, L.K. *et al.*, *Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1*, 1987, 297, *(rev, tox)*
Luxon, S.G.*, Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 653
Lewis, R.J.*, Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HBC500