



>>Entry Name: Octane, 9CI

CAS Registry Number: 111-65-9

Related CAS Registry Numbers(s): 17252-77-6



Molecular Formula: C_8H_{18}

Molecular Weight: 114.23

Accurate Mass: 114.14085

Percentage Composition: C 84.12%; H 15.88%

Biological Source: Found in oil of *Pinus* spp. and in hop oil (*Humulus lupulus*)

Physical Description: Liq.

Melting Point: Fp -56.8°

Boiling Point: Bp 125.67°

Density: d_4^{20} 0.7025

Refractive Index: n_D^{20} 1.3974

Hazard & Toxicity: Eye, skin and respiratory tract irritant. High vapour conc. narcotic. Highly flammable, fl. p. 13° , autoignition temp. $206/210/220^\circ$. OES: long-term 300 ppm; short-term 375 ppm

Aldrich: 41223-6

Fluka: 74823

Sigma: O2001

Supelco: R42-1008

References:

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Whitesides, G.M. *et al.*, *J.A.C.S.*, 1967, **89**, 5302-5303, (synth)

Weil, T.A. *et al.*, *J. Organomet. Chem.*, 1973, **49**, 227-232, (synth)

Kabalka, G.W. *et al.*, *J.O.C.*, 1975, **40**, 1834-1835, (synth)

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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, 307, (rev, tox)

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