



>>Entry Name: Hexadecane

Synonym(s): Cetane

CAS Registry Number: 544-76-3

$\text{H}_3\text{C}(\text{CH}_2)_{14}\text{CH}_3$

Molecular Formula: $\text{C}_{16}\text{H}_{34}$

Molecular Weight: 226.445

Accurate Mass: 226.26605

Percentage Composition: C 84.87%; H 15.13%

Biological Source: Isol. from rose petal oil, oil of *Piper longum* and wood of *Manilkara bidentata*

Use/Importance: Standard for rating diesel-fuel ignition quality

Melting Point: Mp 18.17°

Boiling Point: Bp₁₆₀ 287°. Bp_{0.1} 105-110°

Hazard & Toxicity: Fl. p. >71°, autoignition temp. 202/205°

Aldrich: 29631-7

Fluka: 52210

Sigma: H0255

Supelco: 44-2679

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 4C, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 4A, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 5A, (ir)

Corey, P.C. *et al.*, *J.C.S.*, 1933, 346, (synth)

Org. Synth., 1935, **15**, 27, (synth)

Cocher, W. *et al.*, *J.C.S.*, 1963, 677, (isol)

Niwa, Y. *et al.*, *Bull. Chem. Soc. Jpn.*, 1968, **41**, 1746, (ms)

Tosi, C. *et al.*, *Spectrochim. Acta A*, 1972, **28**, 585, (ir)

Fritz, H. *et al.*, *Chem. Ber.*, 1976, **109**, 1258, (cmr, pmr)