



>>Entry Name: 1-Octyne, 9CI

Synonym(s): Hexylacetylene

CAS Registry Number: 629-05-0

$\text{H}_3\text{C}(\text{CH}_2)_5\text{C}\equiv\text{CH}$

Molecular Formula: C_8H_{14}

Molecular Weight: 110.199

Accurate Mass: 110.10955

Percentage Composition: C 87.20%; H 12.80%

Melting Point: Fp -79.48°

Boiling Point: Bp 126.25°

Density: d_4^{20} 0.746

Refractive Index: n_D^{20} 1.4159

Hazard & Toxicity: Highly flammable, fl. p. 16°

Aldrich: 24446-5

Fluka: 74970

Rare Chemicals Library: S60297-3

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 503A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 932A, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1581B, (*ir*)

Jacobs, T.L., *Org. React. (N.Y.)*, 1949, **5**, 60, (*synth, bibl*)

Weil, L. *et al.*, *Monatsh. Chem.*, 1962, **93**, 952, (*synth*)

Dorman, D.E. *et al.*, *J.O.C.*, 1973, **38**, 1026, (*cmr*)

Smith, W.N. *et al.*, *Synthesis*, 1974, 441, (*synth*)

Sato, F. *et al.*, *Chem. Lett.*, 1978, 789, (*synth*)

Tarchini, C. *et al.*, *Helv. Chim. Acta*, 1979, **62**, 635, (*synth*)

Vinczer, P. *et al.*, *Org. Prep. Proced. Int.*, 1989, **21**, 232, (*synth, pmr*)