



>>Entry Name: 1-Heptyne, 9CI

Synonym(s): Pentylacetylene. Amylacetylene

CAS Registry Number: 628-71-7

$\text{H}_3\text{C}(\text{CH}_2)_4\text{C}\equiv\text{CH}$

Molecular Formula: C_7H_{12}

Molecular Weight: 96.172

Accurate Mass: 96.0939

Percentage Composition: C 87.42%; H 12.58%

Melting Point: Fp -80.93°

Boiling Point: Bp 99.78° (Bp₁₀ 26°)

Hazard & Toxicity: Highly flammable, fl. p. -2°

Aldrich: 24441-4

Fluka: 51950

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **3**, 502C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 931D, (*ir*)

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

Henne, A.L. *et al.*, *J.A.C.S.*, 1945, **67**, 484, (*synth*)

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

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