



>>Entry Name: 1,6-Heptadiyne, 9CI

CAS Registry Number: 2396-63-6

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

Molecular Formula: C_7H_8

Molecular Weight: 92.14

Accurate Mass: 92.0626

Percentage Composition: C 91.25%; H 8.75%

Boiling Point: Bp 112° (resinifies) (109°). Bp₂₆ 30°

Hazard & Toxicity: LD₅₀ (rat, orl) 2300 mg/kg

Aldrich: 40743-7

Rare Chemicals Library: S76477-9

References:

Normant, J.F., *Bull. Soc. Chim. Fr.*, 1965, 859-861, (*synth*)

Smith, W.N. *et al.*, *Synthesis*, 1974, 441-442, (*synth*)

Apping, J.R. *et al.*, *Org. Mass Spectrom.*, 1983, **18**, 292-294, (*ms*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, HAV500