



>>Entry Name: 6-Heptynoic acid

CAS Registry Number: 30964-00-2

$\text{HC}\equiv\text{C}(\text{CH}_2)_4\text{COOH}$

Molecular Formula: $\text{C}_7\text{H}_{10}\text{O}_2$

Molecular Weight: 126.155

Accurate Mass: 126.06808

Percentage Composition: C 66.65%; H 7.99%; O 25.36%

Physical Description: Liq.

Boiling Point: Bp_1 93-94°

Aldrich: 44287-9

Fluka: 51955

>>Derivative: Me ester

Molecular Formula: $\text{C}_8\text{H}_{12}\text{O}_2$

Molecular Weight: 140.182

Accurate Mass: 140.08373

Percentage Composition: C 68.55%; H 8.63%; O 22.83%

Boiling Point: Bp_{11} 80°

>>Derivative: Nitrile

Synonym(s): 6-Heptynenitrile, 9Cl. 6-Cyano-1-hexyne

CAS Registry Number: 15295-69-9

Molecular Formula: $\text{C}_7\text{H}_9\text{N}$

Molecular Weight: 107.155

Accurate Mass: 107.073499

Percentage Composition: C 78.46%; H 8.47%; N 13.07%

Boiling Point: Bp_{14} 87-93°

References:

Taylor, W.R. *et al.*, *J.A.C.S.*, 1950, **72**, 4263, (*synth*)

Ferrier, R.J. *et al.*, *J.C.S.*, 1957, 1435, (*synth, nitrile*)

Gautier, J.A. *et al.*, *Bull. Soc. Chim. Fr.*, 1967, 1551, (*nitrile*)

Moody, C.J. *et al.*, *J.C.S. Perkin I*, 1988, 3249, (*synth, ir, pmr, ms*)