



>>Entry Name: 2-Hexynoic acid, 9CI

Synonym(s): 1-Pentyne-1-carboxylic acid

CAS Registry Number: 764-33-0

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

Molecular Formula:  $\text{C}_6\text{H}_8\text{O}_2$

Molecular Weight: 112.128

Accurate Mass: 112.05243

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Physical Description: Feathery cryst.

Melting Point: Mp 27°

Boiling Point: Bp<sub>16</sub> 119-121°

Solubility: Spar. sol. H<sub>2</sub>O

Other Data: Decarboxylates if dist. at atm. press.

>>Derivative: Me ester

CAS Registry Number: 18937-79-6

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<sub>23</sub> 80-82°

>>Derivative: Et ester

CAS Registry Number: 16205-90-6

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<sub>14</sub> 87-88°

#### References:

Moreau, C. *et al.*, *Bull. Soc. Chim. Fr.*, 1903, **29**, 648

*Org. Synth.*, 1976, **55**, 73, (ester)

Bestman, H.S. *et al.*, *Annalen*, 1977, 282, (synth)

Yamada, K. *et al.*, *Synthesis*, 1977, 679, (ester)