



>>Entry Name: 5-Hexynoic acid

CAS Registry Number: 53293-00-8

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

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: Liq.

Boiling Point: Bp_{20} 120-125°. Bp_6 95-96°

pKa Value: pK_a 4.59 (25°, 0.1M NaCl)

Other Data: Claimed in one paper to be cryst., Mp 41-43.5°

Fluka: 53108

>>Derivative: Me ester

CAS Registry Number: 77758-51-1

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%

Boiling Point: Bp_{10} 56°

>>Derivative: Chloride

CAS Registry Number: 55183-45-4

Molecular Formula: $\text{C}_6\text{H}_7\text{ClO}$

Molecular Weight: 130.573

Accurate Mass: 130.018542

Percentage Composition: C 55.19%; H 5.40%; Cl 27.15%; O 12.25%

Physical Description: Liq.

Boiling Point: $\text{Bp}_{0.5}$ 50-55°

>>Derivative: Nitrile

Synonym(s): 5-Cyano-1-pentyne

CAS Registry Number: 14918-21-9

Molecular Formula: $\text{C}_6\text{H}_7\text{N}$

Molecular Weight: 93.128

Accurate Mass: 93.057849

Percentage Composition: C 77.38%; H 7.58%; N 15.04%

Boiling Point: Bp_7 65.5°

Aldrich: 27134-9

Fluka: 77049

>>Derivative: Anhydride

Molecular Formula: $\text{C}_{12}\text{H}_{14}\text{O}_3$

Molecular Weight: 206.241

Accurate Mass: 206.094295

Percentage Composition: C 69.89%; H 6.84%; O 23.27%

Physical Description: Liq.

Boiling Point: $\text{Bp}_{0.6}$ 122-124°

References: