



>>Entry Name: 5-Hexenoic acid, 9CI
Synonym(s): 4-Pentene-1-carboxylic acid

CAS Registry Number: 1577-22-6
H2C=CH(CH2)3COOH

Molecular Formula: C6H10O2
Molecular Weight: 114.144
Accurate Mass: 114.06808
Percentage Composition: C 63.14%; H 8.83%; O 28.03%
Physical Description: Oil
Boiling Point: Bp₁₀ 93-95°. Bp 203°
pKa Value: pK_a 4.72

Aldrich: 46492-9

>>Derivative: Me ester

CAS Registry Number: 2396-80-7
Molecular Formula: C7H12O2
Molecular Weight: 128.171
Accurate Mass: 128.08373
Percentage Composition: C 65.60%; H 9.44%; O 24.97%
Boiling Point: Bp₁₂ 48°

>>Derivative: Et ester

CAS Registry Number: 54653-25-7
Molecular Formula: C8H14O2
Molecular Weight: 142.197
Accurate Mass: 142.09938
Percentage Composition: C 67.57%; H 9.92%; O 22.50%
Boiling Point: Bp₄ 40°

>>Derivative: Hydrazide

Molecular Formula: C6H12N2O
Molecular Weight: 128.174
Accurate Mass: 128.094963
Percentage Composition: C 56.23%; H 9.44%; N 21.86%; O 12.48%
Melting Point: Mp 46.5-47.5°

>>Derivative: Nitrile
Synonym(s): 5-Cyano-1-pentene

CAS Registry Number: 5048-19-1
Molecular Formula: C6H9N
Molecular Weight: 95.144
Accurate Mass: 95.073499
Percentage Composition: C 75.74%; H 9.53%; N 14.72%
Physical Description: Liq.
Boiling Point: Bp 160-162°

>>Derivative: Anhydride

Molecular Formula: C12H18O3
Molecular Weight: 210.272
Accurate Mass: 210.125595
Percentage Composition: C 68.55%; H 8.63%; O 22.83%
Other Data: No phys. props. given

References: