



>>Entry Name: 2-Pentenoic acid, 9CI
Synonym(s): 1-Butene-1-carboxylic acid

CAS Registry Number: 626-98-2
Related CAS Registry Numbers(s): 818-59-7 13284-42-9 15790-87-1 15856-96-9 18802-94-3
H3CCH2CH=CHCOOH

Molecular Formula: C5H8O2
Molecular Weight: 100.117
Accurate Mass: 100.05243
Percentage Composition: C 59.98%; H 8.05%; O 31.96%

>>Variant: (*E*)-form

CAS Registry Number: 13991-37-2
Molecular Formula: C5H8O2
Molecular Weight: 100.117
Accurate Mass: 100.05243
Percentage Composition: C 59.98%; H 8.05%; O 31.96%
Physical Description: Cryst or liq.
Melting Point: Mp 10°
Boiling Point: Bp₁₇ 108°
Solubility: Mod. sol. H₂O
Density: d¹⁵ 0.992
pKa Value: pK_a 4.74 (25°)
Refractive Index: n_D²⁰ 1.4509
Aldrich: 25927-6
Fluka: 77045

>>Derivative: Me ester

CAS Registry Number: 15790-88-2
Molecular Formula: C6H10O2
Molecular Weight: 114.144
Accurate Mass: 114.06808
Percentage Composition: C 63.14%; H 8.83%; O 28.03%
Physical Description: Liq.
Boiling Point: Bp₂₅ 50-52°

>>Derivative: Et ester

CAS Registry Number: 24410-84-2
Molecular Formula: C7H12O2
Molecular Weight: 128.171
Accurate Mass: 128.08373
Percentage Composition: C 65.60%; H 9.44%; O 24.97%
Physical Description: Liq.
Boiling Point: Bp 157.6°

>>Derivative: *tert*-Butyl ester

CAS Registry Number: 81643-03-0
Molecular Formula: C9H16O2
Molecular Weight: 156.224
Accurate Mass: 156.11503
Percentage Composition: C 69.19%; H 10.32%; O 20.48%
Physical Description: Liq.
Boiling Point: Bp_{0.6} 49-51°