



>>Entry Name: 4-Pentenoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Allylactic acid. 3-Butene-1-carboxylic acid. FEMA 2843

CAS Registry Number: 591-80-0

$\text{H}_2\text{C}=\text{CHCH}_2\text{CH}_2\text{COOH}$

Molecular Formula: $\text{C}_5\text{H}_8\text{O}_2$

Molecular Weight: 100.117

Accurate Mass: 100.05243

Percentage Composition: C 59.98%; H 8.05%; O 31.96%

Use/Importance: Flavouring ingredient

Physical Description: Liq.

Melting Point: Mp -22.5°

Boiling Point: Bp $188-189^\circ$. Bp₄ $70-72^\circ$

Solubility: Sl. sol. H_2O ; sol. EtOH, Et₂O

Density: d_4^{18} 0.984

Refractive Index: n_D^{20} 1.4280

Hazard & Toxicity: LD₅₀ (rat, orl) 470 mg/kg

Aldrich: 24592-5

Fluka: 5950

Rare Chemicals Library: S66231-3

Sigma: P0403

>>Derivative: Me ester

CAS Registry Number: 818-57-5

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_2$

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Physical Description: Liq.

Boiling Point: Bp $128-129^\circ$. Bp₂₂ 42°

>>Derivative: Et ester

CAS Registry Number: 1968-40-7

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}_2$

Molecular Weight: 128.171

Accurate Mass: 128.08373

Percentage Composition: C 65.60%; H 9.44%; O 24.97%

Boiling Point: Bp $144-146^\circ$

Rare Chemicals Library: S94665-6

>>Derivative: 2-Propenyl ester

CAS Registry Number: 75265-78-0

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: Bp₁₂ $83-84^\circ$

Density: d_{20}^{20} 0.9877

Refractive Index: n_D^{20} 1.4280

>>Derivative: Benzyl ester

CAS Registry Number: 113882-48-7

Molecular Formula: $\text{C}_{12}\text{H}_{14}\text{O}_2$

Molecular Weight: 190.241

Accurate Mass: 190.09938

Percentage Composition: C 75.76%; H 7.42%; O 16.82%

Physical Description: Liq.

Boiling Point: Bp₂₅ 137° . Bp₄ $105-106^\circ$