



>>Entry Name: 4-Methyl-2-pentenoic acid, 9CI

Synonym(s): 3-Isopropylacrylic acid

CAS Registry Number: 10321-71-8

$(\text{H}_3\text{C})_2\text{CHCH}=\text{CHCOOH}$

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%

Biological Source: Isol. from hops. Rare occurrence as an esterifying group in terpenoids

pKa Value: $\text{p}K_{\text{a}}$ 4.7 (25°)

>>Variant: (*E*)-form

CAS Registry Number: 16666-43-6

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%

Boiling Point: Bp_3 78°. $\text{Bp}_{0.1}$ 60-64°

>>Derivative: Et ester

CAS Registry Number: 15790-86-0

Molecular Formula: $\text{C}_8\text{H}_{14}\text{O}_2$

Molecular Weight: 142.197

Accurate Mass: 142.09938

Percentage Composition: C 67.57%; H 9.92%; O 22.50%

Boiling Point: Bp 153°. Bp_{17} 66°

>>Derivative: Chloride

CAS Registry Number: 40794-19-2

Molecular Formula: $\text{C}_6\text{H}_9\text{ClO}$

Molecular Weight: 132.589

Accurate Mass: 132.034192

Percentage Composition: C 54.35%; H 6.84%; Cl 26.74%; O 12.07%

Boiling Point: Bp_{25} 61-62°

>>Variant: (*Z*)-form

CAS Registry Number: 1775-44-6

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%

Melting Point: Mp -19°

Boiling Point: $\text{Bp}_{0.4}$ 69-70°

>>Derivative: Et ester

CAS Registry Number: 15790-85-9

Melting Point: Mp 147°

References:

Power, F.B. *et al.*, *J.C.S.*, 1913, **103**, 1267, (*isol*)

Gibson, T.W. *et al.*, *J.O.C.*, 1972, **37**, 1148, (*synth*)

Org. Synth., 1973, **53**, 123, (*synth*)

Pirrung, M.C. *et al.*, *J.O.C.*, 1994, **59**, 2430, (*synth*, *pmr*)