



>>Entry Name: 3-Hydroxy-2,2-dimethylpropanoic acid, 9CI

Synonym(s): Hydroxypivalic acid. Hydroxytrimethylacetic acid. 2,2-Dimethylhydracrylic acid

CAS Registry Number: 4835-90-9

HOCH₂C(CH₃)₂COOH

Molecular Formula: C₅H₁₀O₃

Molecular Weight: 118.132

Accurate Mass: 118.062995

Percentage Composition: C 50.84%; H 8.53%; O 40.63%

Physical Description: Needles (Et₂O/petrol)

Melting Point: Mp 125°

pKa Value: pK_a 4.86

Fluka: 40720

Rare Chemicals Library: S88188-0

>>Derivative: K salt

Physical Description: Cryst.

Melting Point: Mp 234°

>>Derivative: Me ester

CAS Registry Number: 14002-80-3

Molecular Formula: C₆H₁₂O₃

Molecular Weight: 132.159

Accurate Mass: 132.078645

Percentage Composition: C 54.53%; H 9.15%; O 36.32%

Boiling Point: Bp₇₄₀ 177-178°

Aldrich: 22745-5

>>Derivative: Et ester

CAS Registry Number: 14002-73-4

Molecular Formula: C₇H₁₄O₃

Molecular Weight: 146.186

Accurate Mass: 146.094295

Percentage Composition: C 57.51%; H 9.65%; O 32.83%

Boiling Point: Bp₇₅₀ 188°. Bp₃ 70-72°

>>Derivative: 3-Hydroxy-2,2-dimethylpropyl ester

>>Derivative: Nitrile

Synonym(s): 2-Cyano-2-methyl-1-propanol

CAS Registry Number: 19295-57-9

Molecular Formula: C₅H₉NO

Molecular Weight: 99.132

Accurate Mass: 99.068414

Percentage Composition: C 60.58%; H 9.15%; N 14.13%; O 16.14%

Boiling Point: Bp₁₁ 97°

>>Derivative: Et ether

Molecular Formula: C₇H₁₄O₃

Molecular Weight: 146.186

Accurate Mass: 146.094295

Percentage Composition: C 57.51%; H 9.65%; O 32.83%

Boiling Point: Bp₂₂ 123°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1039B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 661D, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 716B, (*ir*)

Johnson, P.Y. *et al.*, *J.O.C.*, 1973, **38**, 2346