



>>Entry Name: **Dipropylpropanedioic acid**, 9CI

Synonym(s): Dipropylmalonic acid, 8CI. Heptane-4,4-dicarboxylic acid

CAS Registry Number: 1636-27-7

$(\text{H}_3\text{CCH}_2\text{CH}_2)_2\text{C}(\text{COOH})_2$

Molecular Formula: $\text{C}_9\text{H}_{16}\text{O}_4$

Molecular Weight: 188.223

Accurate Mass: 188.10486

Percentage Composition: C 57.43%; H 8.57%; O 34.00%

Physical Description: Cryst. (CHCl_3)

Melting Point: Mp 161 dec.°

pKa Value: $\text{p}K_{\text{a}1}$ 1.86; $\text{p}K_{\text{a}2}$ 7.18 (25°, I 0.1 NaClO_4)

>>Derivative: Di-Me ester

CAS Registry Number: 16644-05-6

Molecular Formula: $\text{C}_{11}\text{H}_{20}\text{O}_4$

Molecular Weight: 216.277

Accurate Mass: 216.13616

Percentage Composition: C 61.09%; H 9.32%; O 29.59%

Boiling Point: Bp_{20} 120.5°

>>Derivative: Mono-Et ester

Molecular Formula: $\text{C}_{11}\text{H}_{20}\text{O}_4$

Molecular Weight: 216.277

Accurate Mass: 216.13616

Percentage Composition: C 61.09%; H 9.32%; O 29.59%

Melting Point: Mp 49°

Boiling Point: Bp_{15} 156°

>>Derivative: Di-Et ester

Synonym(s): DEDnPM

CAS Registry Number: 6065-63-0

Molecular Formula: $\text{C}_{13}\text{H}_{24}\text{O}_4$

Molecular Weight: 244.33

Accurate Mass: 244.16746

Percentage Composition: C 63.91%; H 9.90%; O 26.19%

Boiling Point: Bp 249°

Rare Chemicals Library: S36050-3

Other: Hüls

>>Derivative: Dichloride

CAS Registry Number: 56945-52-9

Molecular Formula: $\text{C}_9\text{H}_{14}\text{Cl}_2\text{O}_2$

Molecular Weight: 225.114

Accurate Mass: 224.037084

Percentage Composition: C 48.02%; H 6.27%; Cl 31.50%; O 14.21%

Boiling Point: Bp 221-223°

>>Derivative: Diamide

Molecular Formula: $\text{C}_9\text{H}_{18}\text{N}_2\text{O}_2$

Molecular Weight: 186.253

Accurate Mass: 186.136828

Percentage Composition: C 58.04%; H 9.74%; N 15.04%; O 17.18%

Physical Description: Needles

Melting Point: Mp 214°

Solubility: Mod. sol. hot H_2O

References:

Fürth, H., *Monatsh. Chem.*, 1888, **9**, 318, (*synth*)

Vogel, A.I., *J.C.S.*, 1929, 1478, (*synth*)

Singh, R.K., *Synthesis*, 1985, 54, (*synth, pmr*)