



>>Entry Name: 1,3,5-Pentanetricarboxylic acid, 9CI

Synonym(s): 4-Carboxypimelic acid. Octric acid

CAS Registry Number: 6940-58-5

HOOCCH₂CH₂CH(COOH)CH₂CH₂COOH

Molecular Formula: C₈H₁₂O₆

Molecular Weight: 204.179

Accurate Mass: 204.06339

Percentage Composition: C 47.06%; H 5.92%; O 47.02%

Physical Description: Cryst. (Me₂CO/CHCl₃ or Et₂O)

Melting Point: Mp 116-118°. Mp 208°

pKa Value: pK_{a1} 3.99; pK_{a2} 4.88; pK_{a3} 5.63 (25°)

Rare Chemicals Library: S41966-4

>>Derivative: Tri-Me ester

CAS Registry Number: 5464-63-1

Molecular Formula: C₁₁H₁₈O₆

Molecular Weight: 246.26

Accurate Mass: 246.11034

Percentage Composition: C 53.65%; H 7.37%; O 38.98%

Physical Description: Oil

Boiling Point: Bp₁₂ 162°

>>Derivative: Tri-Et ester

CAS Registry Number: 63579-89-5

Molecular Formula: C₁₄H₂₄O₆

Molecular Weight: 288.34

Accurate Mass: 288.15729

Percentage Composition: C 58.32%; H 8.39%; O 33.29%

Physical Description: Oil

Boiling Point: Bp_{0.001} 120°

>>Derivative: Trinitrile

CAS Registry Number: 4379-04-8

Molecular Formula: C₈H₉N₃

Molecular Weight: 147.179

Accurate Mass: 147.079647

Percentage Composition: C 65.29%; H 6.16%; N 28.55%

Physical Description: Oil

Boiling Point: Bp_{0.5} 190°

>>Derivative: 1,3-Anhydride

Synonym(s): Tetrahydro-2,6-dioxo-2H-pyran-3-propanoic acid, 9CI

CAS Registry Number: 40550-18-3

Molecular Formula: C₈H₁₀O₅

Molecular Weight: 186.164

Accurate Mass: 186.052825

Percentage Composition: C 51.61%; H 5.41%; O 42.97%

Physical Description: Cryst.

Melting Point: Mp 104°

References:

Perkin, W.H. *et al.*, *J.C.S.*, 1896, **69**, 1506-1510; 1900, **77**, 294-309; 1904, **85**, 416-438, (*synth*)

Buchman, E.R. *et al.*, *J.A.C.S.*, 1942, **64**, 2703-2705, (*synth*)

Openshaw, H.T. *et al.*, *J.C.S.*, 1946, 912-918, (*synth*)

Huff, R. *et al.*, *Helv. Chim. Acta*, 1977, **60**, 907-921, (*Et ester, nitrile, synth, ir*)

Waldvogel, S.R. *et al.*, *Helv. Chim. Acta*, 1998, **81**, 46-58, (*anhydride, synth, pmr*)

Suissa, M.R. *et al.*, *Chem. Eur. J.*, 1999, **5**, 3055-3065, (*synth, pmr, cmr, ms*)