



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

Synonym(s): 5-Methylisophthalic acid, 8CI. Toluene-3,5-dicarboxylic acid. Uvitic acid

CAS Registry Number: 499-49-0

Molecular Formula: C₉H₈O₄

Molecular Weight: 180.16

Accurate Mass: 180.04226

Percentage Composition: C 60.00%; H 4.48%; O 35.52%

Physical Description: Needles (H₂O)

Melting Point: Mp 298° (290°)

pKa Value: pK_a 2.53

Rare Chemicals Library: S41997-4

>>Derivative: Di-Me ester

Molecular Formula: C₁₁H₁₂O₄

Molecular Weight: 208.213

Accurate Mass: 208.07356

Percentage Composition: C 63.45%; H 5.81%; O 30.74%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 98°

>>Derivative: Di-Et ester

Molecular Formula: C₁₃H₁₆O₄

Molecular Weight: 236.267

Accurate Mass: 236.10486

Percentage Composition: C 66.09%; H 6.83%; O 27.09%

Physical Description: Cryst.

Melting Point: Mp 35°

Boiling Point: Bp₅ 155-156°

References:

Fittig, R. *et al.*, *Annalen*, 1868, **147**, 292, (*synth*)

Wolff, L. *et al.*, *Annalen*, 1899, **305**, 135, (*synth*)

Schorger, A.W., *J.A.C.S.*, 1917, **39**, 2671, (*synth*)

Schenker, K. *et al.*, *Helv. Chim. Acta*, 1962, **45**, 1344, (*synth*)

Armatage, B.J. *et al.*, *Tetrahedron*, 1964, **20**, 723, (*synth*)