



>>Entry Name: **1,3-Benzenediacetic acid**, 9CI

Synonym(s): 1,3-Bis(carboxymethyl)benzene. *m*-Phenylenediacetic acid. *m*-Xylene- ω,ω' -dicarboxylic acid

CAS Registry Number: 19806-17-8

Molecular Formula: $C_{10}H_{10}O_4$

Molecular Weight: 194.187

Accurate Mass: 194.05791

Percentage Composition: C 61.85%; H 5.19%; O 32.96%

Physical Description: Needles (H_2O)

Melting Point: Mp 170°

Aldrich: P2335-0

>>Derivative: Di-Me ester

CAS Registry Number: 36076-19-4

Molecular Formula: $C_{12}H_{14}O_4$

Molecular Weight: 222.24

Accurate Mass: 222.08921

Percentage Composition: C 64.85%; H 6.35%; O 28.80%

Boiling Point: Bp 298-300°. Bp₁₅ 185-187°

>>Derivative: Di-Et ester

CAS Registry Number: 36076-20-7

Molecular Formula: $C_{14}H_{18}O_4$

Molecular Weight: 250.294

Accurate Mass: 250.12051

Percentage Composition: C 67.18%; H 7.25%; O 25.57%

Boiling Point: Bp₁₂ 188-189°

>>Derivative: Dinitrile

Synonym(s): *m*-Xylylene dicyanide. α,α -Dicyano-*m*-xylene. 1,3-Benzenediacetonitrile. 1,3-Bis(cyanomethyl)benzene

CAS Registry Number: 626-22-2

Molecular Formula: $C_{10}H_8N_2$

Molecular Weight: 156.187

Accurate Mass: 156.068748

Percentage Composition: C 76.90%; H 5.16%; N 17.94%

Physical Description: Cryst.

Melting Point: Mp 28-29°

Boiling Point: Bp₂₅ 170° (lit. gives a pressure range)

Aldrich: P2370-9

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1492B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 153D; 433A, (*ir*)

Titley, A.F., *J.C.S.*, 1928, 2571, (*synth*)

Morton, A.A. *et al.*, *J.A.C.S.*, 1943, **65**, 1339, (*synth*)