



>>Entry Name: 4-Methyl-1,2-benzenedicarboxylic acid, 9CI
Synonym(s): 4-Methylphthalic acid, 8CI. Toluene-3,4-dicarboxylic acid

CAS Registry Number: 4316-23-8

Molecular Formula: $C_9H_8O_4$
Molecular Weight: 180.16
Accurate Mass: 180.04226
Percentage Composition: C 60.00%; H 4.48%; O 35.52%
Physical Description: Cryst. (H_2O)
Melting Point: Mp 152°
pKa Value: pK_{a1} 3.04; pK_{a2} 5.26 (30°, 0.1M KCl)

Aldrich: 34830-9

>>Derivative: Di-Me ester

CAS Registry Number: 20116-65-8
Molecular Formula: $C_{11}H_{12}O_4$
Molecular Weight: 208.213
Accurate Mass: 208.07356
Percentage Composition: C 63.45%; H 5.81%; O 30.74%
Physical Description: Liq.
Boiling Point: Bp₉ 147-151°

>>Derivative: Dinitrile

Synonym(s): 3,4-Dicyanotoluene. 4-Methylphthalonitrile

CAS Registry Number: 63089-50-9
Molecular Formula: $C_9H_6N_2$
Molecular Weight: 142.16
Accurate Mass: 142.053098
Percentage Composition: C 76.04%; H 4.25%; N 19.71%
Physical Description: Needles (H_2O)
Melting Point: Mp 120°
Other Data: Steam-volatile

>>Derivative: 1-Me ester, 2-nitrile

Synonym(s): Methyl 2-cyano-4-methylbenzoate

Molecular Formula: $C_{10}H_9NO_2$
Molecular Weight: 175.187
Accurate Mass: 175.063329
Percentage Composition: C 68.56%; H 5.18%; N 8.00%; O 18.27%
Melting Point: Mp 68°
Boiling Point: Bp 284-290°

>>Derivative: Diamide

CAS Registry Number: 63089-47-4
Molecular Formula: $C_9H_{10}N_2O_2$
Molecular Weight: 178.19
Accurate Mass: 178.074228
Percentage Composition: C 60.66%; H 5.66%; N 15.72%; O 17.96%
Physical Description: Needles
Melting Point: Mp 188°

>>Derivative: Anhydride