



>>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: Bp<sub>9</sub> 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