



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

CAS Registry Number: 37102-74-2

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: Needles (EtOAc)  
Melting Point: Mp 157°

>>Derivative: Dinitrile  
Synonym(s): 2,3-Dicyanotoluene. 3-Methylphthalonitrile

CAS Registry Number: 36715-97-6  
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 (EtOH or  $C_6H_6$ )  
Melting Point: Mp 143°  
Other Data: Steam-volatile

>>Derivative: Di-Me ester

CAS Registry Number: 21483-46-5  
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: Cryst. (MeOH aq.)  
Melting Point: Mp 40-41°  
Boiling Point: Bp<sub>9</sub> 142-147°

>>Derivative: 1-Me ester, 2-nitrile  
Synonym(s): Methyl 2-cyano-3-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%  
Physical Description: Needles (petrol)  
Melting Point: Mp 68-70°

>>Derivative: Diamide

CAS Registry Number: 63089-46-3  
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: Cryst.  
Melting Point: Mp 225°

>>Derivative: Anhydride

CAS Registry Number: 4792-30-7  
Extra CAS Registry Numbers(s): 25134-21-8  
Molecular Formula:  $C_9H_6O_3$   
Molecular Weight: 162.145  
Accurate Mass: 162.031695  
Percentage Composition: C 66.67%; H 3.73%; O 29.60%  
Physical Description: Cryst. (petrol), needles by subl.  
Melting Point: Mp 117-118°