



>>Entry Name: 3-Amino-1,2-benzenedicarboxylic acid, 9CI

Synonym(s): 3-Aminophthalic acid, 8CI

CAS Registry Number: 5434-20-8

Molecular Formula: $C_8H_7NO_4$

Molecular Weight: 181.148

Accurate Mass: 181.037509

Percentage Composition: C 53.04%; H 3.89%; N 7.73%; O 35.33%

Physical Description: Needles (H_2O)

Melting Point: Mp 231-232° (191-192° dec., 187°)

Other Data: Cooling of an aq. soln. gives 3-Aminophthalimidophthalic acid dihydrate, Mp 250-1° (fluorescent)

Aldrich: 33534-7

>>Derivative: Hydrochloride

CAS Registry Number: 6946-22-1

Physical Description: Needles (conc. HCl)

Melting Point: Mp 225 dec.°

Other Data: Softens at 210°

Rare Chemicals Library: S36662-5

Other: PB A27700

>>Derivative: 1-Me ester

CAS Registry Number: 103259-06-9

Molecular Formula: $C_9H_9NO_4$

Molecular Weight: 195.174

Accurate Mass: 195.053159

Percentage Composition: C 55.39%; H 4.65%; N 7.18%; O 32.79%

Physical Description: Cryst. (conc. HCl) (as hydrochloride)

Melting Point: Mp 153 dec.° (as hydrochloride)

>>Derivative: Di-Me ester

CAS Registry Number: 52412-63-2

Molecular Formula: $C_{10}H_{11}NO_4$

Molecular Weight: 209.201

Accurate Mass: 209.068809

Percentage Composition: C 57.41%; H 5.30%; N 6.70%; O 30.59%

Physical Description: Needles (as hydrochloride)

Melting Point: Mp 172-174 dec.° (as hydrochloride)

>>Derivative: Di-Me ester, *N*-Ac

CAS Registry Number: 52659-18-4

Molecular Formula: $C_{12}H_{13}NO_5$

Molecular Weight: 251.238

Accurate Mass: 251.079374

Percentage Composition: C 57.37%; H 5.22%; N 5.58%; O 31.84%

Physical Description: Cryst. (AcOH aq.)

Melting Point: Mp 92-93°

>>Derivative: *N*-Ac

CAS Registry Number: 15371-06-9

Molecular Formula: $C_{10}H_9NO_5$

Molecular Weight: 223.185

Accurate Mass: 223.048074

Percentage Composition: C 53.82%; H 4.06%; N 6.28%; O 35.84%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 206°