



>>Entry Name: 2-Amino-1,4-benzenedicarboxylic acid, 9CI

Synonym(s): Aminoterephthalic acid, 8CI

CAS Registry Number: 10312-55-7

Molecular Formula: C₈H₇NO₄

Molecular Weight: 181.148

Accurate Mass: 181.037509

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

Physical Description: Yellowish cryst. (H₂O)

Melting Point: Mp 324-325 dec.°

pKa Value: pK_a 3.58 (25°)

Other Data: Blue fluor. in soln.

Aldrich: 38107-1

Fluka: 9437

Sigma: A9331

>>Derivative: 1-Me ester

CAS Registry Number: 60728-41-8

Molecular Formula: C₉H₉NO₄

Molecular Weight: 195.174

Accurate Mass: 195.053159

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

Physical Description: Yellow cryst. (MeOH)

Melting Point: Mp 216-217°

Aldrich: 39367-3

>>Derivative: 4-Me ester

CAS Registry Number: 85793-02-8

Molecular Formula: C₉H₉NO₄

Molecular Weight: 195.174

Accurate Mass: 195.053159

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

Physical Description: Needles (MeOH aq.)

Melting Point: Mp 217°