



>>Entry Name: 5-Amino-1,3-benzenedicarboxylic acid, 9CI

Synonym(s): 5-Aminoisophthalic acid, 8CI

CAS Registry Number: 99-31-0

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: Prisms (EtOH)

Melting Point: Mp 300°

Aldrich: 18627-9

Fluka: 8305

>>Derivative: Di-Me ester

CAS Registry Number: 99-27-4

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: Plates (MeOH), pale-yellow cryst.

Melting Point: Mp 176°

Aldrich: D14215-8

Fluka: 8310

Rare Chemicals Library: S41351-8

>>Derivative: N-Ac

CAS Registry Number: 4861-72-7

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: Red needles (H₂O)

Other Data: Dec. at 314-5°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 228A, (*ir*)

Meyer, F. *et al.*, *Ber.*, 1917, **50**, 450, (*synth*)

Loeffler, M. *et al.*, *FEBS Lett.*, 1976, **70**, 76, (*synth*)

Dobson, A.J. *et al.*, *Acta Cryst. C*, 1998, **54**, 1503-1505, (*cryst struct*)