



>>Entry Name: 1,4-Naphthalenedicarboxylic acid, 9Cl, 8Cl

Synonym(s): 1,4-Naphthalic acid

CAS Registry Number: 605-70-9

Molecular Formula: C₁₂H₈O₄

Molecular Weight: 216.193

Accurate Mass: 216.04226

Percentage Composition: C 66.67%; H 3.73%; O 29.60%

Physical Description: Cryst. (AcOH)

Melting Point: Mp 325° (309°)

pKa Value: pK_{a1} 5.36 pK_{a2} 7.12

Other Data: Sol. EtOH → blue fluor.

Aldrich: 33358-1

>>Derivative: Di-Me ester

CAS Registry Number: 7487-15-2

Molecular Formula: C₁₄H₁₂O₄

Molecular Weight: 244.246

Accurate Mass: 244.07356

Percentage Composition: C 68.85%; H 4.95%; O 26.20%

Physical Description: Cryst. (AcOH)

Melting Point: Mp 67°

Boiling Point: Bp₁₂ 195-197°

>>Derivative: Dichloride

CAS Registry Number: 13234-52-1

Molecular Formula: C₁₂H₆Cl₂O₂

Molecular Weight: 253.084

Accurate Mass: 251.974484

Percentage Composition: C 56.95%; H 2.39%; Cl 28.02%; O 12.64%

Physical Description: Needles (petrol)

Melting Point: Mp 80°

>>Derivative: Dinitrile

Synonym(s): 1,4-Dicyanonaphthalene

CAS Registry Number: 3029-30-9

Molecular Formula: C₁₂H₆N₂

Molecular Weight: 178.193

Accurate Mass: 178.053098

Percentage Composition: C 80.89%; H 3.39%; N 15.72%

Use/Importance: Electron acceptor, photosensitiser

Physical Description: Needles (AcOH)

Melting Point: Mp 208°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1171B, (*nmr*)

Scholl, R. *et al.*, *Ber.*, 1922, **55**, 118, (*synth*)

Mayer, F. *et al.*, *Ber.*, 1922, **55**, 1835, (*synth*)

Bradbrook, E.F. *et al.*, *J.C.S.*, 1936, 1739, (*synth*)

Lyssy, T.D. *et al.*, *J.O.C.*, 1962, **27**, 5, (*synth*, *uv*)

Davies, C., *Fuel*, 1973, **52**, 270; 1974, **53**, 105, (*ir*, *uv*)

Albini, A. *et al.*, *Can. J. Chem.*, 1978, **56**, 2985, (*dinitrile*)