



>>Entry Name: 4-Amino-1,8-naphthalenedicarboxylic acid, 9CI

Synonym(s): 4-Aminonaphthalic acid

CAS Registry Number: 18644-22-9

Molecular Formula: C₁₂H₉NO₄

Molecular Weight: 231.207

Accurate Mass: 231.053159

Percentage Composition: C 62.34%; H 3.92%; N 6.06%; O 27.68%

General Statement: Free acid probably unknown

>>Derivative: Di-Me ester

CAS Registry Number: 30084-60-7

Molecular Formula: C₁₄H₁₃NO₄

Molecular Weight: 259.261

Accurate Mass: 259.084459

Percentage Composition: C 64.86%; H 5.05%; N 5.40%; O 24.68%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 86-90°

>>Derivative: Di-Et ester

CAS Registry Number: 30084-58-3

Molecular Formula: C₁₆H₁₇NO₄

Molecular Weight: 287.315

Accurate Mass: 287.115759

Percentage Composition: C 66.89%; H 5.96%; N 4.88%; O 22.27%

Physical Description: Yellow cryst. (EtOH aq.)

Melting Point: Mp 132-132.5°

>>Derivative: Anhydride

CAS Registry Number: 6492-86-0

Molecular Formula: C₁₂H₇NO₃

Molecular Weight: 213.192

Accurate Mass: 213.042594

Percentage Composition: C 67.61%; H 3.31%; N 6.57%; O 22.51%

Physical Description: Orange needles (PhNO₂)

Melting Point: Mp 350°

Aldrich: 23559-8

>>Derivative: Anhydride, N-Ac

Molecular Formula: C₁₄H₉NO₄

Molecular Weight: 255.229

Accurate Mass: 255.053159

Percentage Composition: C 65.88%; H 3.55%; N 5.49%; O 25.07%

Physical Description: Cryst. (AcOH)

Melting Point: Mp 282-283°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 336A, (*ir*)

Graebe, C. *et al.*, *Annalen*, 1903, **327**, 77

Okazaki, M. *et al.*, *CA*, 1957, **51**, 8051

Jones, L.A. *et al.*, *Can. J. Chem.*, 1970, **48**, 3132