



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

Synonym(s): 3-Amino-2-naphthoic acid, 8CI

CAS Registry Number: 5959-52-4

Molecular Formula: $C_{11}H_9NO_2$

Molecular Weight: 187.198

Accurate Mass: 187.063329

Percentage Composition: C 70.58%; H 4.85%; N 7.48%; O 17.09%

Use/Importance: Azo dyestuff intermediate, used in detection of Cu, Ni, Co

Physical Description: Yellow leaflets (EtOH aq.)

Melting Point: Mp 219-220° (214°)

Solubility: Spar. sol. hot H₂O

Other Data: Fluor. in soln.

Hazard & Toxicity: LD₅₀ (mus, orl) 1600 mg/kg

Aldrich: A6680-4

Fluka: 8660

>>Derivative: Me ester

CAS Registry Number: 21597-54-6

Molecular Formula: $C_{12}H_{11}NO_2$

Molecular Weight: 201.224

Accurate Mass: 201.078979

Percentage Composition: C 71.63%; H 5.51%; N 6.96%; O 15.90%

Melting Point: Mp 104-105°

>>Derivative: Et ester

Molecular Formula: $C_{13}H_{13}NO_2$

Molecular Weight: 215.251

Accurate Mass: 215.094629

Percentage Composition: C 72.54%; H 6.09%; N 6.51%; O 14.87%

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 117-118°

>>Derivative: N-Ac

Molecular Formula: $C_{13}H_{11}NO_3$

Molecular Weight: 229.235

Accurate Mass: 229.073894

Percentage Composition: C 68.11%; H 4.84%; N 6.11%; O 20.94%

Physical Description: Prisms (EtOH aq.)

Melting Point: Mp 246°

References:

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **2**, 1172B, (nmr)

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Fierz-David, H.E. *et al.*, *Helv. Chim. Acta*, 1922, **5**, 557, (synth)

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Mentre, I. *et al.*, *Bull. Soc. Chim. Fr.*, 1972, 2605, (uv, bibl)

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