



>>Entry Name: **1*H*-Indole-5-carboxylic acid**

CAS Registry Number: 1670-81-1

Molecular Formula: C₉H₇NO₂

Molecular Weight: 161.16

Accurate Mass: 161.047679

Percentage Composition: C 67.08%; H 4.38%; N 8.69%; O 19.86%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 208-209°

pKa Value: p*K*_{a2} 16.92 (25°,NH, KOH aq.)

Aldrich: I-540-0

Fluka: 57230

Sigma: I2250

>>**Derivative:** Me ester

CAS Registry Number: 1011-65-0

Molecular Formula: C₁₀H₉NO₂

Molecular Weight: 175.187

Accurate Mass: 175.063329

Percentage Composition: C 68.56%; H 5.18%; N 8.00%; O 18.27%

Melting Point: Mp 65-66°

>>**Derivative:** Nitrile

Synonym(s): 5-Cyanoindole

CAS Registry Number: 15861-24-2

Molecular Formula: C₉H₆N₂

Molecular Weight: 142.16

Accurate Mass: 142.053098

Percentage Composition: C 76.04%; H 4.25%; N 19.71%

Melting Point: Mp 104-105°

Aldrich: C9200-6

Fluka: 28495

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 139C; 158C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 668C; 678B, (*ir*)

Singer, H. *et al.*, *J.O.C.*, 1955, **20**, 1458

Ikan, R. *et al.*, *Tetrahedron*, 1967, **23**, 3823, (*synth*)

Gassman, P.G. *et al.*, *J.A.C.S.*, 1974, **96**, 5495, (*synth*)

Clark, R.D. *et al.*, *J. Het. Chem.*, 1985, **22**, 121, (*nitrile*)

Russell, H.F. *et al.*, *Org. Prep. Proced. Int.*, 1985, **17**, 391, (*nitrile*)