



>>Entry Name: **1*H*-Indole-7-carboxylic acid**

CAS Registry Number: 1670-83-3

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. (EtOH aq.)

Melting Point: Mp 198-199°

Rare Chemicals Library: S31845-0

>>Derivative: Me ester

CAS Registry Number: 93247-78-0

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 44-45°

>>Derivative: Nitrile

Synonym(s): 7-Cyanoindole

CAS Registry Number: 96631-87-7

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 96°

References:

Singer, H. *et al.*, *J.A.C.S.*, 1955, **77**, 5700

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

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

Norman, M.H. *et al.*, *J. Med. Chem.*, 1996, **39**, 4692-4703, (*synth, pmr, cmr*)