



>>Entry Name: 3-Methyl-1*H*-indole-2-carboxylic acid, 9CI

Synonym(s): Skatole-2-carboxylic acid

CAS Registry Number: 10590-73-5

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%

Physical Description: Needles (AcOH)

Melting Point: Mp 164-165°

Solubility: Sol. EtOH, Et₂O, C₆H₆, spar. sol. H₂O, petrol

>>Derivative: Me ester

CAS Registry Number: 104711-29-7

Molecular Formula: C₁₁H₁₁NO₂

Molecular Weight: 189.213

Accurate Mass: 189.078979

Percentage Composition: C 69.83%; H 5.86%; N 7.40%; O 16.91%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 148°

>>Derivative: Et ester

CAS Registry Number: 26304-51-8

Molecular Formula: C₁₂H₁₃NO₂

Molecular Weight: 203.24

Accurate Mass: 203.094629

Percentage Composition: C 70.92%; H 6.45%; N 6.89%; O 15.74%

Physical Description: Needles (EtOH)

Melting Point: Mp 133-134°

Solubility: Sol. Et₂O, C₆H₆

References:

Perkin, W.H. *et al.*, *J.C.S.*, 1921, **119**, 1602-1642, (*synth*)

Whalley, W.B., *J.C.S.*, 1954, 1651-1653, (*synth*)

Andrisano, R. *et al.*, *Gazz. Chim. Ital.*, 1957, **87**, 949-970, (*uv*)

Jones, C.D., *J.O.C.*, 1972, **37**, 3624-3625, (*synth*)

Wadia, M.S. *et al.*, *Synthesis*, 1987, 401-404, (*Et ester, synth, ir, pmr*)

Katritzky, A.R. *et al.*, *Synth. Commun.*, 1988, **18**, 1151-1158, (*Me ester, synth, ir, pmr*)

Murakami, Y. *et al.*, *Chem. Pharm. Bull.*, 1997, **45**, 1739-1744, (*Et ester, synth, ir, pmr*)