



>>Entry Name: 2,5-Dimethyl-1*H*-indole, 9Cl

CAS Registry Number: 1196-79-8

Structure by analogy with 2,3-Dimethyl-1*H*-indole, [FWS76-L](#)

Molecular Formula: C₁₀H₁₁N

Molecular Weight: 145.204

Accurate Mass: 145.089149

Percentage Composition: C 82.72%; H 7.64%; N 9.65%

Physical Description: Cryst.

Melting Point: Mp 114-115°

Boiling Point: Bp₄₀ 188°

pKa Value: pK_a 0.26 (25°, H₂SO₄ aq.)

Aldrich: D16600-6

>>Derivative: Picrate

Physical Description: Red needles (C₆H₆)

Melting Point: Mp 159°

>>Derivative: *N*-Me

Synonym(s): 1,2,5-Trimethyl-1*H*-indole

CAS Registry Number: 53711-77-6

Molecular Formula: C₁₁H₁₃N

Molecular Weight: 159.23

Accurate Mass: 159.104799

Percentage Composition: C 82.97%; H 8.23%; N 8.80%

Physical Description: Leaflets (EtOH aq.)

Melting Point: Mp 56-57°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 124B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 655C, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1499C, (*ir*)

Bayer, A., *Chem. Zentralbl.*, 1903, **1**, 109, (*synth, deriv*)

Marion, L. *et al.*, *Can. J. Res., Sect. B*, 1947, **25**, 1, (*synth*)

Ger. Pat., 1974, 2 412 509; *CA*, **82**, 113184z, (*N-Me*)

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

McDonald, B.G. *et al.*, *J.C.S. Perkin I*, 1975, 1446, (*synth*)