



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

Synonym(s): α -Methylindole

CAS Registry Number: 95-20-5

Molecular Formula: C₉H₉N

Molecular Weight: 131.177

Accurate Mass: 131.073499

Percentage Composition: C 82.41%; H 6.92%; N 10.68%

Source/Synthesis: Found in coal tar

Physical Description: Needles (H₂O), plates (EtOH aq.)

Melting Point: Mp 61°

Boiling Point: Bp 271-272°

Solubility: Sol. EtOH, Et₂O; spar. sol. hot H₂O

pK_a Value: pK_a -0.28 (25°, H₂SO₄ aq.)

Other Data: Triboluminescent. Solns. fluor. viol. to blue-green in daylight. Heat in sealed tube → quinoline.

Aldrich: M5140-7

Fluka: 67600

Sigma: M2002

>>Derivative: Picrate

Physical Description: Brown-red needles

Melting Point: Mp 139°

>>Derivative: *N*-Formyl

Molecular Formula: C₁₀H₉NO

Molecular Weight: 159.187

Accurate Mass: 159.068414

Percentage Composition: C 75.45%; H 5.70%; N 8.80%; O 10.05%

Physical Description: Plates

Melting Point: Mp 75-76°

Boiling Point: Bp₁₅ 155°

Density: d₄¹⁶ 1.135

Refractive Index: n_D¹⁶ 1.6170

>>Derivative: *N*-Ac

Molecular Formula: C₁₁H₁₁NO

Molecular Weight: 173.214

Accurate Mass: 173.084064

Percentage Composition: C 76.28%; H 6.40%; N 8.09%; O 9.24%

Boiling Point: Bp₄₀ 200-210°

>>Derivative: *N*-Me

Synonym(s): 1,2-Dimethyl-1*H*-indole, 9CI

CAS Registry Number: 875-79-6

Molecular Formula: C₁₀H₁₁N

Molecular Weight: 145.204

Accurate Mass: 145.089149

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

Physical Description: Needles (petrol)

Melting Point: Mp 56°

Boiling Point: Bp_{1.2} 85-89°

Solubility: Spar. sol. hot H₂O

pK_a Value: pK_a 0.34 (25°, H₂SO₄ aq.)

Aldrich: D16560-3

References: