



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

ENTRY UNDER REVIEW

CAS Registry Number: 625-84-3

Structure by analogy with 2,3-Dimethyl-1*H*-pyrrole, [FWW15-M](#)

Molecular Formula: C₆H₉N

Molecular Weight: 95.144

Accurate Mass: 95.073499

Percentage Composition: C 75.74%; H 9.53%; N 14.72%

Physical Description: Oil

Boiling Point: Bp₇₆₀ 165°. Bp₈ 50-53°

Solubility: Prac. insol. H₂O

Density: d₄²⁰ 0.935

Refractive Index: n_D²⁰ 1.5036

Other Data: Steam-volatile.

Hazard & Toxicity: LD₅₀ (rat, orl) 59 mg/kg

Aldrich: D18360-1

>>Derivative: *N*-Ac

Synonym(s): 1-Acetyl-2,5-dimethyl-1*H*-pyrrole

CAS Registry Number: 5044-31-5

Molecular Formula: C₈H₁₁NO

Molecular Weight: 137.181

Accurate Mass: 137.084064

Percentage Composition: C 70.04%; H 8.08%; N 10.21%; O 11.66%

Boiling Point: Bp₂₇ 122-125°

>>Derivative: *N*-Me

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

CAS Registry Number: 930-87-0

Molecular Formula: C₇H₁₁N

Molecular Weight: 109.171

Accurate Mass: 109.089149

Percentage Composition: C 77.01%; H 10.16%; N 12.83%

Physical Description: Liq.

Boiling Point: Bp₇₄₆ 169°. Bp₉ 55-56°

pK_a Value: pK_a -0.24

Aldrich: T8030-6

>>Derivative: *N*-Et

Synonym(s): 1-Ethyl-2,5-dimethylpyrrole

CAS Registry Number: 5044-19-9

Molecular Formula: C₈H₁₃N

Molecular Weight: 123.197

Accurate Mass: 123.104799

Percentage Composition: C 78.00%; H 10.64%; N 11.37%

Physical Description: Liq.

Boiling Point: Bp₇₃₉ 174°. Bp₄₅ 103.5-104.5°

Refractive Index: n_D²⁰ 1.4884

>>Derivative: *N*-Benzyl

CAS Registry Number: 5044-20-2

Molecular Formula: C₁₃H₁₅N

Molecular Weight: 185.268

Accurate Mass: 185.120449

Percentage Composition: C 84.28%; H 8.16%; N 7.56%

Physical Description: Pale yellow cryst. solid

Melting Point: Mp 40-41°

References: