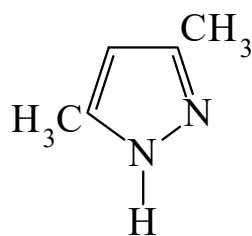




>>Entry Name: 3,5-Dimethyl-1*H*-pyrazole, 9Cl



CAS Registry Number: 67-51-6

Type of Compound Code(s): PA1450 PS8300

Molecular Formula: C₅H₈N₂

Molecular Weight: 96.132

Accurate Mass: 96.068748

Percentage Composition: C 62.47%; H 8.39%; N 29.14%

Use/Importance: Used in photometric detn. of Cu (with use of SCN⁽⁻⁾). Forms CrO₃ complex used for oxidn. of alcohols

Physical Description: Cryst. (petrol)

Melting Point: Mp 106-107°

Boiling Point: Bp 218°

Solubility: Sol. H₂O

pKa Value: p*K*_a 4.12 (20°)

Other Data: Steam-volatile

Aldrich: D18200-1

Fluka: 41540

>>Derivative: Picrate

Melting Point: Mp 166-167°

>>Variant: 1*H*-form

Molecular Formula: C₅H₈N₂

Molecular Weight: 96.132

Accurate Mass: 96.068748

Percentage Composition: C 62.47%; H 8.39%; N 29.14%

>>Derivative: *N*-Ac

Molecular Formula: C₇H₁₀N₂O

Molecular Weight: 138.169

Accurate Mass: 138.079313

Percentage Composition: C 60.85%; H 7.29%; N 20.27%; O 11.58%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 38°

Boiling Point: Bp₄₀ 88-90°

>>Derivative: *N*-Benzoyl

Molecular Formula: C₁₂H₁₂N₂O

Molecular Weight: 200.24

Accurate Mass: 200.094963

Percentage Composition: C 71.98%; H 6.04%; N 13.99%; O 7.99%

Physical Description: Needles (EtOH)

Melting Point: Mp 48-49°