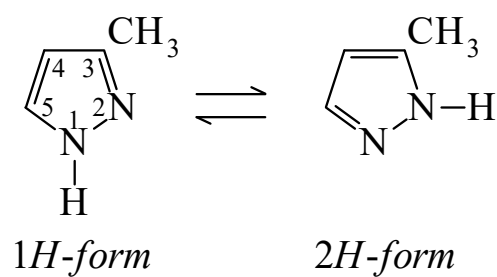




>>Entry Name: 3(5)-Methylpyrazole, 9CI



Related CAS Registry Numbers(s): 79210-25-6 79554-60-2

Molecular Formula: C₄H₆N₂

Molecular Weight: 82.105

Accurate Mass: 82.053098

Percentage Composition: C 58.52%; H 7.37%; N 34.12%

Physical Description: Liq.

Boiling Point: Bp₇₃₀ 204-205°. Bp₁ 72°

Solubility: Misc. H₂O, EtOH, Et₂O

Density: d₄²⁰ 1.022

pKa Value: pK_a 3.32 (25°, H₂O)

Refractive Index: n_D²⁰ 1.4968

Other Data: Spar. steam-volatile

Hazard & Toxicity: LD₅₀ (rat, orl) 1000 mg/kg

>>Derivative: Picrate

CAS Registry Number: 14710-76-0

Physical Description: Needles

Melting Point: Mp 144° (141°)

Solubility: V. sol. H₂O

>>Variant: 1*H*-form

CAS Registry Number: 1453-58-3

Molecular Formula: C₄H₆N₂

Molecular Weight: 82.105

Accurate Mass: 82.053098

Percentage Composition: C 58.52%; H 7.37%; N 34.12%

Aldrich: M7580-2

Fluka: 69015

>>Derivative: *N*¹-Ac

CAS Registry Number: 69413-00-9

Molecular Formula: C₆H₈N₂O

Molecular Weight: 124.142

Accurate Mass: 124.063663

Percentage Composition: C 58.05%; H 6.50%; N 22.57%; O 12.89%

Physical Description: Prisms (petrol)

Melting Point: Mp 29-30°

Boiling Point: Bp₁₀ 70-71°

>>Derivative: *N*¹-Benzoyl

CAS Registry Number: 69413-11-2

Molecular Formula: C₁₁H₁₀N₂O

Molecular Weight: 186.213

Accurate Mass: 186.079313

Percentage Composition: C 70.95%; H 5.41%; N 15.04%; O 8.59%

Boiling Point: Bp₁₄ 155-157°

>>Derivative: *N*¹-2-Nitrobenzoyl