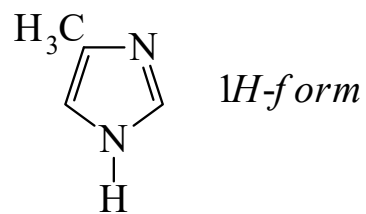




>>Entry Name: 4(5)-Methylimidazole, 9CI



CAS Registry Number: 822-36-6

Molecular Formula: C₄H₆N₂

Molecular Weight: 82.105

Accurate Mass: 82.053098

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

Biological Source: Isol. from flowers of *Sophora flavescens*

Physical Description: Cryst.

Melting Point: Mp 56°

Boiling Point: Bp 263°. Bp_{0.2} 120-125°

Solubility: Sol. H₂O, EtOH

pKa Value: pK_a 7.52 (25°)

Other Data: Prob. an artifact

Hazard & Toxicity: LD₅₀ (mus, orl) 370 mg/kg

Aldrich: 19988-5

Fluka: 67580

Sigma: M3019

>>Derivative: Picrate

Physical Description: Yellow cryst. (H₂O)

Melting Point: Mp 159-160°

>>Variant: 1*H*-form

Molecular Formula: C₄H₆N₂

Molecular Weight: 82.105

Accurate Mass: 82.053098

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

>>Derivative: 1-Benzoyl

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%

Physical Description: Needles

Melting Point: Mp 54-55°

Solubility: V. sol. EtOH, Me₂CO, C₆H₆, sol. petrol

>>Derivative: 1-Me

Synonym(s): 1,4-Dimethyl-1*H*-imidazole

CAS Registry Number: 6338-45-0

Molecular Formula: C₅H₈N₂

Molecular Weight: 96.132

Accurate Mass: 96.068748

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

Boiling Point: Bp 198-200°

>>Derivative: 1-Me; hydrochloride

Molecular Formula: C₅H₉ClN₂

Molecular Weight: 132.592

Percentage Composition: C 45.29%; H 6.84%; Cl 26.74%; N 21.13%

Melting Point: Mp 168-169°