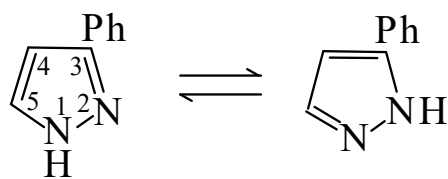




>>Entry Name: 3(5)-Phenylpyrazole



CAS Registry Number: 2458-26-6

Molecular Formula: C₉H₈N₂

Molecular Weight: 144.176

Accurate Mass: 144.068748

Percentage Composition: C 74.98%; H 5.59%; N 19.43%

Physical Description: Needles (H₂O)

Melting Point: Mp 79°

Boiling Point: Bp 313-314°. Bp₁₁ 177-178°

Solubility: Sol. EtOH, Et₂O

pKa Value: pK_a 2.13 (20°)

Hazard & Toxicity: LD₅₀ (mus, orl) 500 mg/kg

Rare Chemicals Library: S94528-5

>>Variant: 1*H*-form

Molecular Formula: C₉H₈N₂

Molecular Weight: 144.176

Accurate Mass: 144.068748

Percentage Composition: C 74.98%; H 5.59%; N 19.43%

>>Derivative: *N*-Ac

CAS Registry Number: 38858-98-9

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 (petrol)

Melting Point: Mp 64-65°

Boiling Point: Bp₁₀ 157-158°

Solubility: Sol. Me₂CO, C₆H₆; spar. sol. EtOH, petrol

>>Derivative: *N*-Ethoxycarbonyl

Molecular Formula: C₁₂H₁₂N₂O₂

Molecular Weight: 216.239

Accurate Mass: 216.089878

Percentage Composition: C 66.65%; H 5.59%; N 12.95%; O 14.80%

Physical Description: Oil

Boiling Point: Bp₁₃ 193°

>>Derivative: *N*-(2-Nitrobenzoyl)

Physical Description: Cryst. (MeOH)

Melting Point: Mp 107.5-108.5°

Solubility: Sol. Me₂CO, C₆H₆; spar. sol. MeOH

>>Derivative: *N*-Me

Synonym(s): 1-Methyl-3-phenyl-1*H*-pyrazole, 9CI

CAS Registry Number: 3463-26-1

Molecular Formula: C₁₀H₁₀N₂

Molecular Weight: 158.202

Accurate Mass: 158.084398

Percentage Composition: C 75.92%; H 6.37%; N 17.71%

Melting Point: Mp 56°

Boiling Point: Bp 280-281°. Bp₁₂ 138-139°