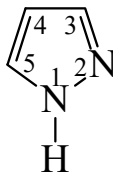




>>Entry Name: Pyrazole, 9CI, 8CI

Synonym(s): 1,2-Diazole



CAS Registry Number: 288-13-1

Molecular Formula: C₃H₄N₂

Molecular Weight: 68.078

Accurate Mass: 68.037448

Percentage Composition: C 52.93%; H 5.92%; N 41.15%

at r.t.

Physical Description: Needles or prisms (petrol)

Melting Point: Mp 69.5-70°

Boiling Point: Bp_{757.900024} 186-188°

Solubility: Sol. H₂O, EtOH, Et₂O, C₆H₆

pKa Value: pK_{a1} 2.52; pK_{a2} 14.21 (25°)

Other Data: No tautomerism present in cryst. state at r.t.

Hazard & Toxicity: LD₅₀ (rat, ori) 1010 mg/kg. Exp. reprod. and teratogenic effects

Aldrich: P5660-7

Fluka: 82620

Sigma: P2646

>>Derivative: Hydrochloride

CAS Registry Number: 35877-22-6

Physical Description: Hygroscopic needles

Melting Point: Mp 104°

>>Derivative: Sulfate (2:1)

Physical Description: Cryst. (EtOH)

Melting Point: Mp 134°

>>Derivative: Nitrate

Physical Description: Needles

Melting Point: Mp 148°

>>Derivative: *N*-Ac

CAS Registry Number: 10199-64-1

Molecular Formula: C₅H₆N₂O

Molecular Weight: 110.115

Accurate Mass: 110.048013

Percentage Composition: C 54.54%; H 5.49%; N 25.44%; O 14.53%

Physical Description: Oil

Boiling Point: Bp₇₄₄ 155-156°

>>Derivative: *N*-Benzoyl

CAS Registry Number: 10199-66-3

Molecular Formula: C₁₀H₈N₂O

Molecular Weight: 172.186

Accurate Mass: 172.063663

Percentage Composition: C 69.76%; H 4.68%; N 16.27%; O 9.29%

Melting Point: Mp 46°

Boiling Point: Bp₇₄₇ 281°. Bp₁₁ 140°

>>Derivative: *N*-Me