



>>Entry Name: 4-Phenylpyrazole, 9CI

CAS Registry Number: 10199-68-5

Molecular Formula:  $C_9H_8N_2$

Molecular Weight: 144.176

Accurate Mass: 144.068748

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

Physical Description: Plates (EtOH)

Melting Point: Mp 230°

Solubility: Sol. EtOH,  $C_6H_6$ ; spar. sol.  $Et_2O$

>>Derivative: *N*-Ac

CAS Registry Number: 40711-89-5

Molecular Formula:  $C_{11}H_{10}N_2O$

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 ( $Et_2O$  or MeOH)

Melting Point: Mp 82°

>>Derivative: *N*-Benzoyl

CAS Registry Number: 40711-91-9

Molecular Formula:  $C_{16}H_{12}N_2O$

Molecular Weight: 248.284

Accurate Mass: 248.094963

Percentage Composition: C 77.40%; H 4.87%; N 11.28%; O 6.44%

Physical Description: Plates ( $Et_2O$ )

Melting Point: Mp 128-129°

>>Derivative: *N*-Me

Synonym(s): 1-Methyl-4-phenyl-1*H*-pyrazole, 9CI

CAS Registry Number: 10199-69-6

Molecular Formula:  $C_{10}H_{10}N_2$

Molecular Weight: 158.202

Accurate Mass: 158.084398

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

Physical Description: Cryst.

Melting Point: Mp 102-102.5°

>>Derivative: *N*-Ph

Synonym(s): 1,4-Diphenyl-1*H*-pyrazole, 9CI

CAS Registry Number: 15132-01-1

Molecular Formula:  $C_{15}H_{12}N_2$

Molecular Weight: 220.273

Accurate Mass: 220.100048

Percentage Composition: C 81.79%; H 5.49%; N 12.72%

Physical Description: Yellowish leaflets (EtOH aq.)

Melting Point: Mp 97°

Solubility: Sol.  $Et_2O$ ,  $C_6H_6$ , petrol

References: