



Boiling Point: Bp_{0.25} 130°

>> **Derivative:** 1-Ph

Synonym(s): 3-Amino-1-phenylpyrazole

CAS Registry Number: 1128-56-9

Molecular Formula: C₉H₉N₃

Molecular Weight: 159.19

Accurate Mass: 159.079647

Percentage Composition: C 67.91%; H 5.70%; N 26.40%

Melting Point: Mp 162-164° (as hydrochloride)

pKa Value: pK_a 2.66

>> **Variant:** 2H-form

Molecular Formula: C₃H₅N₃

Molecular Weight: 83.093

Accurate Mass: 83.048347

Percentage Composition: C 43.36%; H 6.06%; N 50.57%

>> **Derivative:** 2-Me

Synonym(s): 5-Amino-1-methylpyrazole

CAS Registry Number: 1192-21-8

Molecular Formula: C₄H₇N₃

Molecular Weight: 97.119

Accurate Mass: 97.063997

Percentage Composition: C 49.47%; H 7.26%; N 43.27%

pKa Value: pK_a 4.23 (25°, H₂O)

>> **Derivative:** 2-Me; hydrochloride

CAS Registry Number: 32016-34-5

Melting Point: Mp 141-143°

>> **Derivative:** 2-Me, picrate

CAS Registry Number: 1904-34-3

Physical Description: Large yellow prisms (MeOH)

Melting Point: Mp 221-224°

>> **Derivative:** 2-Ph

Synonym(s): 5-Amino-1-phenylpyrazole

CAS Registry Number: 826-85-7

Molecular Formula: C₉H₉N₃

Molecular Weight: 159.19

Accurate Mass: 159.079647

Percentage Composition: C 67.91%; H 5.70%; N 26.40%

Melting Point: Mp 182-185 dec.° (as hydrochloride)

pKa Value: pK_a 3.23

Rare Chemicals Library: S43807-3

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **3**, 69C, (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 607D, (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1482B, (*ir*)
Org. Synth., 1968, **48**, 8, (*synth*)
Cusack, N.J. *et al.*, *J.C.S.(C)*, 1971, 1501, (*derivs*)
Dorn, H. *et al.*, *J. Prakt. Chem.*, 1973, **315**, 382, (*tautom*)
Ege, G. *et al.*, *Synthesis*, 1976, 52, (*synth, pmr, derivs*)
Catalán, J. *et al.*, *J. Het. Chem.*, 1985, **22**, 997, (*props*)
Garrone, A. *et al.*, *J.C.S. Perkin 2*, 1989, 1941, (*N-15 nmr, derivs*)