



>>Entry Name: 4-Aminopyrazole
Synonym(s): 1*H*-Pyrazol-4-amine, 9CI

CAS Registry Number: 28466-26-4

Molecular Formula: C₃H₅N₃
Molecular Weight: 83.093
Accurate Mass: 83.048347
Percentage Composition: C 43.36%; H 6.06%; N 50.57%
Melting Point: Mp 80-82°
pKa Value: p*K*_a 5.57 (25°, H₂O)
Other Data: Hygroscopic, sublimes, dimorphic

>>Derivative: Picrate

Melting Point: Mp 193-196°

>>Derivative: 4,4-Di-*N*-benzoyl

Molecular Formula: C₁₇H₁₃N₃O₂
Molecular Weight: 291.309
Accurate Mass: 291.100777
Percentage Composition: C 70.09%; H 4.50%; N 14.42%; O 10.98%
Physical Description: Cryst. (EtOH)
Melting Point: Mp 173°

>>Derivative: 1-Me

Synonym(s): 4-Amino-1-methylpyrazole

Molecular Formula: C₄H₇N₃
Molecular Weight: 97.119
Accurate Mass: 97.063997
Percentage Composition: C 49.47%; H 7.26%; N 43.27%
pKa Value: p*K*_a 5.52 (25°, H₂O)

>>Derivative: 1-Ph

Synonym(s): 4-Amino-1-phenylpyrazole

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 250-252 dec.° (as hydrochloride)
pKa Value: p*K*_a 4.6

References:

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Ruscia, M., *Ann. Chim. (Rome)*, 1959, **49**, 720
Dorn, H. *et al.*, *J. Prakt. Chem.*, 1973, **315**, 382, (*tautom*)
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*)
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