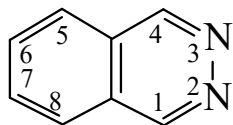




>>Entry Name: Phthalazine, 9Cl, 8Cl

Synonym(s): 2,3-Diazanaphthalene. 2,3-Naphthyridine. β -Phenodiazine. 2,3-Benzodiazine



CAS Registry Number: 253-52-1

Molecular Formula: $C_8H_6N_2$

Molecular Weight: 130.149

Accurate Mass: 130.053098

Percentage Composition: C 73.83%; H 4.65%; N 21.52%

Physical Description: Needles (Et_2O)

Melting Point: Mp 89-92°

Boiling Point: Bp₂₉ 189°. Bp₁₇ 175°

Solubility: Sol. H_2O , EtOH, C_6H_6 ; spar. sol. Et_2O ; insol. petrol

pKa Value: pK_a 3.47 (20°, H_2O)

Aldrich: P3870-6

>>Derivative: Hydroiodide

Melting Point: Mp 203°

>>Derivative: Methiodide

CAS Registry Number: 38710-51-9

Physical Description: Bright yellow cryst.

Melting Point: Mp 243-244 dec.°

>>Derivative: Ethiodide

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 225-228 dec.° (204-210°)

>>Derivative: 2-Me, picrate

Physical Description: Orange cryst. (EtOH)

Melting Point: Mp 199-200 dec.°

>>Derivative: 2-Et, picrate

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 167-169 dec.°

>>Derivative: 2-Oxide

CAS Registry Number: 18636-89-0

Molecular Formula: $C_8H_6N_2O$

Molecular Weight: 146.148

Accurate Mass: 146.048013

Percentage Composition: C 65.75%; H 4.14%; N 19.17%; O 10.95%

Melting Point: Mp 143°

Other Data: Forms a hydrate, Mp 94°

References:

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **3**, 464B, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 880D, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1573C, (ir)

Paul, Y., Ber., 1899, **32**, 2014, (synth)

Smith, R.F. et al., J.O.C., 1962, **27**, 879; 4372, (synth, deriv)

Black, P.J. et al., Aust. J. Chem., 1965, **18**, 707, (pmr)

Bowie, J.H. et al., Aust. J. Chem., 1967, **20**, 2677, (ms)

Huiszoon, C. et al., Acta Cryst. B, 1972, **28**, 3415, (cryst struct)

Patel, N.R., Heteroat. Chem., (ed. Castle R.N.), Wiley, New York, 1973, **27**, 323, (rev)

van de Weijer, P. et al., Org. Magn. Reson., 1976, **8**, 187, (cmr)

Nguyen, M. et al., J.O.C., 1990, **55**, 6177, (synth)