



>>Entry Name: 4-Phenylpyrimidine, 9CI

CAS Registry Number: 3438-48-0

Molecular Formula: C₁₀H₈N₂

Molecular Weight: 156.187

Accurate Mass: 156.068748

Percentage Composition: C 76.90%; H 5.16%; N 17.94%

Physical Description: Needles (hexane), leaflets (MeOH aq.)

Melting Point: Mp 66°

Boiling Point: Bp₄ 117°

Aldrich: P3380-1

>>Derivative: Picrate

Melting Point: Mp 142-143°

>>Derivative: 1-Oxide

CAS Registry Number: 14161-40-1

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 133-135°

>>Derivative: 3-Oxide

CAS Registry Number: 52816-79-2

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 153-155°

>>Derivative: 1,3-Dioxide

CAS Registry Number: 56642-53-6

Molecular Formula: C₁₀H₈N₂O₂

Molecular Weight: 188.185

Accurate Mass: 188.058578

Percentage Composition: C 63.83%; H 4.28%; N 14.89%; O 17.00%

Melting Point: Mp 216-218°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 807B, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 359B, (*nmr*)

Bredereck, H. *et al.*, *Chem. Ber.*, 1960, **93**, 1402, (*synth*)

Ditchfield, R. *et al.*, *J.C.S.(A)*, 1969, 533, (*pmr*)

Wagner, R.M. *et al.*, *Chem. Ber.*, 1971, **104**, 2975, (*synth*)

Kato, T. *et al.*, *Org. Mass Spectrom.*, 1974, **9**, 981, (*ms*)

Boesveld, W.M. *et al.*, *J.C.S. Perkin 1*, 2001, 1103-1108, (*synth, pmr, cmr*)