



>>Entry Name: 4-Methylpyrimidine, 9CI

CAS Registry Number: 3438-46-8

Molecular Formula: C₅H₆N₂

Molecular Weight: 94.116

Accurate Mass: 94.053098

Percentage Composition: C 63.81%; H 6.43%; N 29.76%

Physical Description: Oil

Boiling Point: Bp₇₅₀ 141°

Solubility: Misc. H₂O

Density: d_{15,9}¹⁶ 1.03

pKa Value: pK_a 1.91 (20°)

Aldrich: 12749-3

Fluka: 69080

Sigma: M8262

>>Derivative: Picrate

CAS Registry Number: 30537-72-5

Physical Description: Plates or needles (MeOH)

Melting Point: Mp 131-132°

>>Derivative: Methiodide

CAS Registry Number: 22292-58-6

Melting Point: Mp 111-112°

>>Derivative: 1-Oxide

CAS Registry Number: 17758-54-2

Molecular Formula: C₅H₆N₂O

Molecular Weight: 110.115

Accurate Mass: 110.048013

Percentage Composition: C 54.54%; H 5.49%; N 25.44%; O 14.53%

Melting Point: Mp 74-78°

References:

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

Paudler, W.W. *et al.*, *Org. Magn. Reson.*, 1971, **3**, 217, (*nmr*)

Peerboome, R. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1974, **93**, 58, (*deriv*)

Ernst, L., *Angew. Chem.*, 1976, **88**, 335, (*cmr*)

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