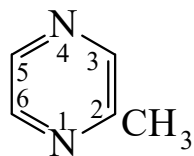




>>Entry Name: Methylpyrazine, 9CI, 8CI
ENTRY UNDER REVIEW



CAS Registry Number: 109-08-0

Molecular Formula: C₅H₆N₂
Molecular Weight: 94.116
Accurate Mass: 94.053098
Percentage Composition: C 63.81%; H 6.43%; N 29.76%
Use/Importance: Flavouring agent
Physical Description: Liq. with disagreeable picoline-like odour
Boiling Point: Bp 136-137°
Solubility: Misc. H₂O, EtOH, Et₂O
Density: d₄²⁰ 1.029
pKa Value: pK_{a1} 1.41; pK_{a2} -4.89 (25°, H₂O)
Refractive Index: n_D²⁰ 1.4953
Hazard & Toxicity: Emits highly toxic fumes when heated to dec. Flammable, fl. p. 50° (oc)

Aldrich: W33090-6
Fluka: 69000

>>Derivative: Picrate

Physical Description: Yellow prisms (EtOH)
Melting Point: Mp 133°

>>Derivative: Methiodide

CAS Registry Number: 34260-05-4
Physical Description: Leaflets and needles (EtOH)
Melting Point: Mp 129-130°
Solubility: V. sol. H₂O

>>Derivative: 1-Oxide

CAS Registry Number: 31396-35-7
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 93-95°

>>Derivative: 4-Oxide

CAS Registry Number: 25594-37-0
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 69-71°

>>Derivative: 1,4-Dioxide

CAS Registry Number: 32046-26-7
Molecular Formula: C₅H₆N₂O₂
Molecular Weight: 126.115
Accurate Mass: 126.042928
Percentage Composition: C 47.62%; H 4.80%; N 22.21%; O 25.37%
Physical Description: Cryst. (MeOH)
Melting Point: Mp 230-231°

References: