



>>Entry Name: 1*H*-Imidazole-4(5)-carboxaldehyde, 9CI

Synonym(s): 4-Formylimidazole

CAS Registry Number: 3034-50-2

Molecular Formula: C₄H₄N₂O

Molecular Weight: 96.088

Accurate Mass: 96.032363

Percentage Composition: C 50.00%; H 4.20%; N 29.15%; O 16.65%

Melting Point: Mp 174-175° (169°)

Aldrich: 45612-8

>>Derivative: Oxime

CAS Registry Number: 57090-90-1

Molecular Formula: C₄H₅N₃O

Molecular Weight: 111.103

Accurate Mass: 111.043262

Percentage Composition: C 43.24%; H 4.54%; N 37.82%; O 14.40%

Physical Description: Prisms (EtOH)

Melting Point: Mp 183-184°

>>Derivative: 4-Methylphenylhydrazone

CAS Registry Number: 17049-92-2

Physical Description: Prisms

Melting Point: Mp 186-188 dec.°

>>Variant: 1*H*-form

Molecular Formula: C₄H₄N₂O

Molecular Weight: 96.088

Accurate Mass: 96.032363

Percentage Composition: C 50.00%; H 4.20%; N 29.15%; O 16.65%

>>Derivative: *N*-Me

Synonym(s): 1-Methyl-1*H*-imidazole-5-carboxaldehyde, 9CI

CAS Registry Number: 39021-62-0

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%

Physical Description: Solid by subl.

Melting Point: Mp 54-55° (52-53°)

References:

Link, H. *et al.*, *Helv. Chim. Acta*, 1972, **55**, 1053, (*N*-Me)

Ferris, J.P. *et al.*, *J.O.C.*, 1976, **41**, 19, (*oxime*, *ir*, *pmr*)

Battersby, A.R. *et al.*, *J.C.S. Perkin I*, 1980, 43

Kirk, K.L., *J. Het. Chem.*, 1985, **22**, 57, (*synth*)

Dener, J.M. *et al.*, *J.O.C.*, 1993, **58**, 1159, (*N*-Me, *synth*, *pmr*, *cmr*)

Winter, J. *et al.*, *Synthesis*, 1994, 245, (*synth*)

Schwarz, M.W. *et al.*, *Synthesis*, 1994, 247, (*N*-Me)