



Accurate Mass: 112.027278

Percentage Composition: C 42.86%; H 3.60%; N 24.99%; O 28.55%

>>>**Derivative:** 1-Me

Synonym(s): 1-Methyl-1*H*-imidazole-4-carboxylic acid

CAS Registry Number: 41716-18-1

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%

Melting Point: Mp 246-247 dec.°

>>>**Derivative:** 1-Me, Me ester

Molecular Formula: C₆H₈N₂O₂

Molecular Weight: 140.141

Accurate Mass: 140.058578

Percentage Composition: C 51.42%; H 5.75%; N 19.99%; O 22.83%

Melting Point: Mp 103-104°

>>>**Variant:** 3*H*-form

Molecular Formula: C₄H₄N₂O₂

Molecular Weight: 112.088

Accurate Mass: 112.027278

Percentage Composition: C 42.86%; H 3.60%; N 24.99%; O 28.55%

>>>**Derivative:** 3-Me

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

CAS Registry Number: 41806-40-0

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%

Melting Point: Mp 256-257 (245-248°) dec.°

>>>**Derivative:** 3-Me, Me ester

Molecular Formula: C₆H₈N₂O₂

Molecular Weight: 140.141

Accurate Mass: 140.058578

Percentage Composition: C 51.42%; H 5.75%; N 19.99%; O 22.83%

Physical Description: Prisms (MeOH)

Melting Point: Mp 68-70° (54-56°)

References:

Balaban, I.E., *J.C.S.*, 1930, 270

Heubner, C.F. *et al.*, *J.A.C.S.*, 1949, **71**, 2801, (*synth*)

Onishchuk, A.E., *J. Gen. Chem. USSR (Engl. Transl.)*, 1955, **25**, 949; *CA*, **50**, 3412

Takahashi, K. *et al.*, *Bull. Chem. Soc. Jpn.*, 1980, **53**, 557, (*1-Me, 3-Me*)

Mitsunashi, K. *et al.*, *J. Het. Chem.*, 1983, **20**, 1103, (*nitrile, synth, pmr, ir*)

Matthews, D.P. *et al.*, *J.O.C.*, 1986, **51**, 3228, (*nitrile, ir, pmr*)

Leone-Bay, A. *et al.*, *Synth. Commun.*, 1987, **17**, 1409, (*nitrile*)

O'Connell, J.F. *et al.*, *Synthesis*, 1988, 767, (*synth, ir, pmr, cmr, 3-Me*)