



>>Entry Name: 4-Formyl-1*H*-pyrrole-2-carboxylic acid

CAS Registry Number: 7126-53-6

Structure by analogy with 2-Formyl-1*H*-pyrrole-3-carboxylic acid, [CXV19-L](#)

Molecular Formula: C₆H₅NO₃

Molecular Weight: 139.11

Accurate Mass: 139.026944

Percentage Composition: C 51.80%; H 3.62%; N 10.07%; O 34.50%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 220°

>>Derivative: Et ester

CAS Registry Number: 7126-57-0

Molecular Formula: C₈H₉NO₃

Molecular Weight: 167.164

Accurate Mass: 167.058244

Percentage Composition: C 57.48%; H 5.43%; N 8.38%; O 28.71%

Physical Description: Cryst. (petrol)

Melting Point: Mp 104-106°

Boiling Point: Bp_{0.1} 115-136°

>>Derivative: Isopropyl ester

Molecular Formula: C₉H₁₁NO₃

Molecular Weight: 181.191

Accurate Mass: 181.073894

Percentage Composition: C 59.66%; H 6.12%; N 7.73%; O 26.49%

Physical Description: Cryst. (toluene/cyclohexane)

Melting Point: Mp 85-86°

References:

Davies, W.A. *et al.*, *Tetrahedron*, 1962, **18**, 405, (*ester*)

Khan, M.K.A. *et al.*, *Tetrahedron*, 1966, **22**, 2095, (*synth, ir, pmr*)

Alonso Garrido, D.O. *et al.*, *J.O.C.*, 1988, **53**, 403, (*synth, cmr*)

Wallace, D.M. *et al.*, *J.O.C.*, 1993, **58**, 7245, (*Et ester*)

Artico, M. *et al.*, *J. Med. Chem.*, 2000, **43**, 1886-1891, (*isopropyl ester*)