



>>Entry Name: 5-Phenyl-1*H*-pyrrole-3-carboxylic acid, 9CI

Molecular Formula: C₁₁H₉NO₂

Molecular Weight: 187.198

Accurate Mass: 187.063329

Percentage Composition: C 70.58%; H 4.85%; N 7.48%; O 17.09%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 206-208 (180°) dec.°

>>Derivative: Et ester

Molecular Formula: C₁₃H₁₃NO₂

Molecular Weight: 215.251

Accurate Mass: 215.094629

Percentage Composition: C 72.54%; H 6.09%; N 6.51%; O 14.87%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 149-151°

>>Derivative: Nitrile

Synonym(s): 4-Cyano-2-phenylpyrrole

CAS Registry Number: 122453-85-4

Molecular Formula: C₁₁H₈N₂

Molecular Weight: 168.198

Accurate Mass: 168.068748

Percentage Composition: C 78.55%; H 4.79%; N 16.66%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 161-163°

References:

Blicke, F.F. *et al.*, *J.A.C.S.*, 1944, **66**, 1675

Di Santo, R. *et al.*, *Synth. Commun.*, 1995, **25**, 795, (*nitrile, Et ester*)