



>>Entry Name: **1*H*-Pyrrole-3-carboxylic acid**, 9CI

CAS Registry Number: 931-03-3

Molecular Formula: C₅H₅NO₂

Molecular Weight: 111.1

Accurate Mass: 111.032029

Percentage Composition: C 54.05%; H 4.54%; N 12.61%; O 28.80%

Physical Description: Needles (EtOAc)

Melting Point: Mp 150-150.5°

pKa Value: p*K*_{a1} 5 (20°) p*K*_a 4.95

Other Data: Decarboxylates on heating *in vacuo*

>>Derivative: Me ester

CAS Registry Number: 2703-17-5

Molecular Formula: C₆H₇NO₂

Molecular Weight: 125.127

Accurate Mass: 125.047679

Percentage Composition: C 57.59%; H 5.64%; N 11.19%; O 25.57%

Physical Description: Needles or leaflets

Melting Point: Mp 87°

Solubility: Sol. EtOH, Et₂O

>>Derivative: Et ester

CAS Registry Number: 37964-17-3

Molecular Formula: C₇H₉NO₂

Molecular Weight: 139.154

Accurate Mass: 139.063329

Percentage Composition: C 60.42%; H 6.52%; N 10.07%; O 23.00%

Physical Description: Cryst. (petrol)

Melting Point: Mp 40°. Mp 49°

>>Derivative: Nitrile

Synonym(s): 1*H*-Pyrrole-3-carbonitrile, 9CI. 3-Cyanopyrrole

CAS Registry Number: 7126-38-7

Molecular Formula: C₅H₄N₂

Molecular Weight: 92.1

Accurate Mass: 92.037448

Percentage Composition: C 65.21%; H 4.38%; N 30.42%

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 56-56.5°

>>Derivative: *N*¹-Ph

Synonym(s): 1-Phenyl-1*H*-pyrrole-3-carboxylic acid

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. (Et₂O/petrol)

Melting Point: Mp 126° (119-120°)

>>Derivative: *N*¹-Ph, Me ester

CAS Registry Number: 85111-36-0

Molecular Formula: C₁₂H₁₁NO₂

Molecular Weight: 201.224

Accurate Mass: 201.078979

Percentage Composition: C 71.63%; H 5.51%; N 6.96%; O 15.90%

Physical Description: Cryst. (hexane/Et₂O)

Melting Point: Mp 82°