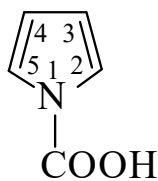




>>Entry Name: 1*H*-Pyrrole-1-carboxylic acid, 9CI



CAS Registry Number: 21972-99-6

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: Prisms (Et₂O)

Melting Point: Mp 95 dec.°. Mp 118°

Other Data: Decarboxylates at Mp. Resinifies with min. acids

>>Derivative: Me ester

CAS Registry Number: 4277-63-8

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: Liq.

Boiling Point: Bp 168-170°. Bp₁₂ 50-50.5°

Aldrich: 42399-8

>>Derivative: Et ester

CAS Registry Number: 4277-64-9

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: Liq.

Boiling Point: Bp₇₇₀ 180°. Bp₁₂ 65°

>>Derivative: *tert*-Butyl ester

Synonym(s): *N-tert*-Butyloxycarbonylpyrrole

CAS Registry Number: 5176-27-2

Molecular Formula: C₉H₁₃NO₂

Molecular Weight: 167.207

Accurate Mass: 167.094629

Percentage Composition: C 64.65%; H 7.84%; N 8.38%; O 19.14%

Physical Description: Liq.

Boiling Point: Bp₁₀ 79-80°

Aldrich: 42583-4

>>Derivative: Ph ester

CAS Registry Number: 56880-01-4

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. (hexane)

Melting Point: Mp 45-46°