



>>Entry Name: **1*H*-Indole-4-carboxylic acid**, 9CI

CAS Registry Number: 2124-55-2

Molecular Formula: C₉H₇NO₂

Molecular Weight: 161.16

Accurate Mass: 161.047679

Percentage Composition: C 67.08%; H 4.38%; N 8.69%; O 19.86%

Melting Point: Mp 213-214°

Aldrich: 24626-3

Sigma: I6257

>>Derivative: Me ester

CAS Registry Number: 39830-66-5

Molecular Formula: C₁₀H₉NO₂

Molecular Weight: 175.187

Accurate Mass: 175.063329

Percentage Composition: C 68.56%; H 5.18%; N 8.00%; O 18.27%

Melting Point: Mp 64°

Aldrich: 27388-0

Fluka: 57236

>>Derivative: Et ester

CAS Registry Number: 50614-84-1

Molecular Formula: C₁₁H₁₁NO₂

Molecular Weight: 189.213

Accurate Mass: 189.078979

Percentage Composition: C 69.83%; H 5.86%; N 7.40%; O 16.91%

Melting Point: Mp 70-71°

Sigma: I6132

>>Derivative: Nitrile

Synonym(s): 4-Cyanoindole

CAS Registry Number: 16136-52-0

Molecular Formula: C₉H₆N₂

Molecular Weight: 142.16

Accurate Mass: 142.053098

Percentage Composition: C 76.04%; H 4.25%; N 19.71%

Melting Point: Mp 120-121°

>>Derivative: *N*-Me

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

Molecular Formula: C₁₀H₉NO₂

Molecular Weight: 175.187

Accurate Mass: 175.063329

Percentage Composition: C 68.56%; H 5.18%; N 8.00%; O 18.27%

Physical Description: Needles (Me₂CO aq.)

Melting Point: Mp 243°

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

Molecular Formula: C₁₁H₁₁NO₂

Molecular Weight: 189.213

Accurate Mass: 189.078979

Percentage Composition: C 69.83%; H 5.86%; N 7.40%; O 16.91%

Physical Description: Flakes (Et₂O/petrol)

Melting Point: Mp 53°

>>Derivative: *N*-Benzyl