



>>Entry Name: **1*H*-Indole-6-carboxylic acid**, 9CI

CAS Registry Number: 1670-82-2

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%

Physical Description: Cryst. (AcOH)

Melting Point: Mp 243-245°

Fluka: 57235

>>Derivative: Me ester

CAS Registry Number: 50820-65-0

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 78-79°

>>Derivative: Nitrile

Synonym(s): 6-Cyanoindole

CAS Registry Number: 15861-36-6

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 129-130°

>>Derivative: *N*-Me

Synonym(s): 1-Methyl-1*H*-indole-6-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 190°

>>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: Plates (MeOH aq.)

Melting Point: Mp 89°

>>Derivative: *N*-Me, nitrile

Synonym(s): 6-Cyano-1-methylindole

Molecular Formula: C₁₀H₈N₂

Molecular Weight: 156.187

Accurate Mass: 156.068748

Percentage Composition: C 76.90%; H 5.16%; N 17.94%

Physical Description: Cryst. (Et₂O/petrol)

Melting Point: Mp 55°

References: