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

CAS Registry Number: 1670-82-2

Molecular Formula: $C_9H_7NO_2$
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: $C_{10}H_9NO_2$
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: $C_9H_6N_2$
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: $C_{10}H_9NO_2$
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 (Me_2CO aq.)
Melting Point: Mp 190°

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

Molecular Formula: $C_{11}H_{11}NO_2$
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: $C_{10}H_8N_2$
Molecular Weight: 156.187
Accurate Mass: 156.068748
Percentage Composition: C 76.90%; H 5.16%; N 17.94%
Physical Description: Cryst. (Et_2O/petrol)
Melting Point: Mp 55°

References: