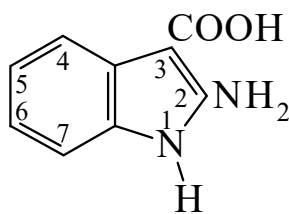




>>Entry Name: 2-Amino-1*H*-indole-3-carboxylic acid, 9CI



Molecular Formula: C₉H₈N₂O₂

Molecular Weight: 176.174

Accurate Mass: 176.058578

Percentage Composition: C 61.36%; H 4.58%; N 15.90%; O 18.16%

>>Derivative: Me ester

CAS Registry Number: 113772-14-8

Molecular Formula: C₁₀H₁₀N₂O₂

Molecular Weight: 190.201

Accurate Mass: 190.074228

Percentage Composition: C 63.15%; H 5.30%; N 14.73%; O 16.82%

Physical Description: Cryst.

Melting Point: Mp 135-137°

>>Derivative: Et ester

CAS Registry Number: 6433-72-3

Molecular Formula: C₁₁H₁₂N₂O₂

Molecular Weight: 204.228

Accurate Mass: 204.089878

Percentage Composition: C 64.69%; H 5.92%; N 13.72%; O 15.67%

Physical Description: Cryst. (C₆H₆); leaflets (C₆H₆/petrol)

Melting Point: Mp 180-181°

>>Derivative: Benzyl ester

Molecular Formula: C₁₆H₁₄N₂O₂

Molecular Weight: 266.299

Accurate Mass: 266.105528

Percentage Composition: C 72.17%; H 5.30%; N 10.52%; O 12.02%

Physical Description: Solid (EtOH)

Melting Point: Mp 166-167°

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

CAS Registry Number: 113772-15-9

Molecular Formula: C₁₁H₁₂N₂O₂

Molecular Weight: 204.228

Accurate Mass: 204.089878

Percentage Composition: C 64.69%; H 5.92%; N 13.72%; O 15.67%

Physical Description: Brown needles (MeOH)

Melting Point: Mp 192-196°

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

CAS Registry Number: 55643-99-7

Molecular Formula: C₁₂H₁₄N₂O₂

Molecular Weight: 218.255

Accurate Mass: 218.105528

Percentage Composition: C 66.04%; H 6.47%; N 12.84%; O 14.66%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 137-139°