



>>Entry Name: 6-Hydroxy-1*H*-indole-2-carboxylic acid, 9CI

CAS Registry Number: 40047-23-2

Molecular Formula: C₉H₇NO₃

Molecular Weight: 177.159

Accurate Mass: 177.042594

Percentage Composition: C 61.02%; H 3.98%; N 7.91%; O 27.09%

Physical Description: Needles (H₂O)

Melting Point: Mp 236 dec.°

>>Derivative: Et ester

CAS Registry Number: 15050-03-0

Molecular Formula: C₁₁H₁₁NO₃

Molecular Weight: 205.213

Accurate Mass: 205.073894

Percentage Composition: C 64.38%; H 5.40%; N 6.83%; O 23.39%

Physical Description: Cryst. (EtOH aq. or C₆H₆)

Melting Point: Mp 179-180°

>>Derivative: *O*-Benzyl

CAS Registry Number: 40047-22-1

Molecular Formula: C₁₆H₁₃NO₃

Molecular Weight: 267.284

Accurate Mass: 267.089544

Percentage Composition: C 71.90%; H 4.90%; N 5.24%; O 17.96%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 200 dec.°

>>Derivative: Me ether

Synonym(s): 6-Methoxy-1*H*-indole-2-carboxylic acid

CAS Registry Number: 16732-73-3

Molecular Formula: C₁₀H₉NO₃

Molecular Weight: 191.186

Accurate Mass: 191.058244

Percentage Composition: C 62.82%; H 4.74%; N 7.33%; O 25.11%

Physical Description: Sandy cryst.

Melting Point: Mp 196-197°

Other Data: Decarboxylates above Mp

>>Derivative: Me ether, Me ester

CAS Registry Number: 98081-83-5

Molecular Formula: C₁₁H₁₁NO₃

Molecular Weight: 205.213

Accurate Mass: 205.073894

Percentage Composition: C 64.38%; H 5.40%; N 6.83%; O 23.39%

Melting Point: Mp 117-119°

Aldrich: 36557-2

>>Derivative: Me ether, *tert*-butyl ester

Molecular Formula: C₁₄H₁₇NO₃

Molecular Weight: 247.293

Accurate Mass: 247.120844

Percentage Composition: C 68.00%; H 6.93%; N 5.66%; O 19.41%

Physical Description: Needles (C₆H₆/hexane)

Melting Point: Mp 153-155°

References: