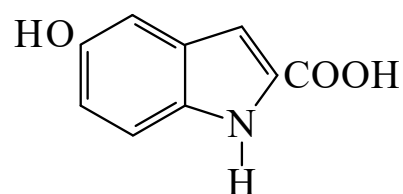




>>Entry Name: 5-Hydroxy-1*H*-indole-2-carboxylic acid, 9CI



CAS Registry Number: 21598-06-1

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%

Use/Importance: Used for photometric detn. of NO₂⁽⁻⁾ ($\lambda_{\max}$ 465 nm, ϵ 3500, H₂SO₄)

Melting Point: Mp 246 dec.°

Aldrich: 14351-0

Fluka: 55355

Sigma: H6509

>>Derivative: Me ester

CAS Registry Number: 51991-39-0

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: Plates (MeOH)

Melting Point: Mp 177°

>>Derivative: Et ester

CAS Registry Number: 24985-85-1

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: Needles (EtOH)

Melting Point: Mp 156°

>>Derivative: Me ether

Synonym(s): 5-Methoxy-1*H*-indole-2-carboxylic acid

CAS Registry Number: 4382-54-1

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: Needles (H₂O)

Melting Point: Mp 196-197 dec.°

Solubility: Sol. EtOH, Et₂O, AcOH

pKa Value: p*K*_{a2} 17.03 (25°,NH)

Hazard & Toxicity: LD₅₀ (mus, ipr) 350 mg/kg

Aldrich: M1495-1

Fluka: 65010

Sigma: M6637