



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

Synonym(s): Indoxylic acid. Indogenic acid

CAS Registry Number: 6245-93-8

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: Cryst.

Other Data: Sublimes with dec. at 122-3°. Oxid. → Indigotin. Heat → indoxyl

>>Derivative: Me ester

CAS Registry Number: 31827-04-0

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: Needles (MeOH)

Melting Point: Mp 157-158°

Rare Chemicals Library: S95544-2

>>Derivative: Me ester, 3-Ac

CAS Registry Number: 77941-13-0

Molecular Formula: C₁₂H₁₁NO₄

Molecular Weight: 233.223

Accurate Mass: 233.068809

Percentage Composition: C 61.80%; H 4.75%; N 6.01%; O 27.44%

Melting Point: Mp 145°

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

Molecular Formula: C₁₂H₁₁NO₄

Molecular Weight: 233.223

Accurate Mass: 233.068809

Percentage Composition: C 61.80%; H 4.75%; N 6.01%; O 27.44%

Melting Point: Mp 124-126°

>>Derivative: Et ester

CAS Registry Number: 14370-74-2

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 120-121°

>>Derivative: Me ether

CAS Registry Number: 21598-04-9

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%

Melting Point: Mp 127-130°

>>Derivative: Et ether

CAS Registry Number: 70258-73-0

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%

Melting Point: Mp 160°