



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

CAS Registry Number: 152213-40-6

Related CAS Registry Numbers(s): 147539-80-8

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%

Physical Description: Plates (H₂O)

Melting Point: Mp 271°

Other Data: Dec. on standing in air

>>Derivative: Et ester

CAS Registry Number: 71086-99-2

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: Light orange needles (C₆H₆)

Melting Point: Mp 127-127.5°

>>Derivative: *N*-Ac

CAS Registry Number: 199805-80-6

Molecular Formula: C₁₁H₁₀N₂O₃

Molecular Weight: 218.212

Accurate Mass: 218.069143

Percentage Composition: C 60.55%; H 4.62%; N 12.84%; O 22.00%

Physical Description: Powder

Melting Point: Mp 260 dec.°

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

CAS Registry Number: 110887-42-8

Molecular Formula: C₁₃H₁₄N₂O₃

Molecular Weight: 246.265

Accurate Mass: 246.100443

Percentage Composition: C 63.40%; H 5.73%; N 11.38%; O 19.49%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 202-203°

References:

Lindwall, H.G. *et al.*, *J.O.C.*, 1953, **18**, 345, (*synth*)

Katti, H.A. *et al.*, *Indian J. Chem., Sect. B*, 1983, **22**, 1205, (*Et ester, synth*)

Warpehoski, M.A. *et al.*, *J. Med. Chem.*, 1988, **31**, 590, (*Et ester*)

Wang, Y. *et al.*, *J. Med. Chem.*, 2000, **43**, 1541-1549, (*N-Ac*)