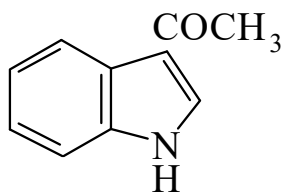




>>Entry Name: 3-Acetylindole

Synonym(s): 1-(1*H*-Indol-3-yl)ethanone, 9CI. 3-Indolyl methyl ketone



CAS Registry Number: 703-80-0

Related CAS Registry Numbers(s): 40747-12-4 40747-13-5

Molecular Formula: C₁₀H₉NO

Molecular Weight: 159.187

Accurate Mass: 159.068414

Percentage Composition: C 75.45%; H 5.70%; N 8.80%; O 10.05%

Physical Description: Cryst. (cyclohexane/EtOH)

Melting Point: Mp 194°

Solubility: Spar. sol. H₂O

pKa Value: p*K*_a 12.99 (25°,NH)

Hazard & Toxicity: LD₅₀ (mus, ipr) 300 mg/kg

Aldrich: A1680-7

Fluka: 1220

Sigma: A9750

>>Derivative: Picrate

Physical Description: Yellow cryst. (petrol)

Melting Point: Mp 183°

>>Derivative: *N*-Ac

Molecular Formula: C₁₂H₁₁NO₂

Molecular Weight: 201.224

Accurate Mass: 201.078979

Percentage Composition: C 71.63%; H 5.51%; N 6.96%; O 15.90%

Melting Point: Mp 151°

Solubility: Sol. hot H₂O

Other Data: Sublimes

>>Derivative: Oxime

Molecular Formula: C₁₀H₁₀N₂O

Molecular Weight: 174.202

Accurate Mass: 174.079313

Percentage Composition: C 68.95%; H 5.79%; N 16.08%; O 9.18%

Melting Point: Mp 144-147°

>>Derivative: *N*-Me

Synonym(s): 3-Acetyl-1-methylindole

Molecular Formula: C₁₁H₁₁NO

Molecular Weight: 173.214

Accurate Mass: 173.084064

Percentage Composition: C 76.28%; H 6.40%; N 8.09%; O 9.24%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 104-105°

References: