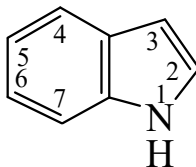




>>Entry Name: Indole, 9CI, 8CI

ENTRY UNDER REVIEW

Synonym(s): 1-Benzazole. 2,3-Benzopyrrole. 1-Azaindene. Ketole (obsol.). FEMA 2593



CAS Registry Number: 120-72-9

Molecular Formula: C₈H₇N

Molecular Weight: 117.15

Accurate Mass: 117.057849

Percentage Composition: C 82.02%; H 6.02%; N 11.96%

Biological Source: Constit. of several flower oils, esp. of *Jasminum* and *Citrus* spp. (Oleaceae, Rutaceae). A prod. of bacterial dec. of proteins, ubiquitous in faeces. Also a constit. of coal tar. Constit. of anal gland secretion of aardwolf *Proteles cristatus*

Use/Importance: Perfumery and flavouring ingredient. Used as 0.5% EtOH soln. for photometric detn. of NO₂⁽⁻⁾. λ_{max} 530 nm (ε 9500, 2.5-5M HCl)

Physical Description: Cryst. (H₂O)

Melting Point: Mp 52°

Boiling Point: Bp 253-254°. Bp₅ 122.5-124°

Solubility: Sol. EtOH; BERDY SOL: Sol. MeOH, Et₂O; poorly sol. H₂O

pKa Value: pK_{a1} -2.4; pK_{a2} 16.97 (25°,NH, KOH aq.)

UV: [neutral] λ_{max} 216 (); 270 (); 278 (); 281 (); 295 () (MeOH) (Berdy)

Hazard & Toxicity: LD₅₀ (rat, orl) 1000 mg/kg

Aldrich: 26907-7

Fluka: 57190

Sigma: I0750

Supelco: R30-0630

>>Derivative: N-Formyl

Molecular Formula: C₉H₇NO

Molecular Weight: 145.16

Accurate Mass: 145.052764

Percentage Composition: C 74.47%; H 4.86%; N 9.65%; O 11.02%

Melting Point: Mp 52°

Boiling Point: Bp₈ 125-126°

>>Derivative: N-Ac

CAS Registry Number: 576-15-8

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%

Boiling Point: Bp₁₄ 152-153°

Aldrich: 37710-4

Rare Chemicals Library: S36626-9

>>Derivative: N-Benzenesulfonyl

CAS Registry Number: 40899-71-6

Molecular Formula: C₁₄H₁₁NO₂S

Molecular Weight: 257.312

Accurate Mass: 257.051049

Percentage Composition: C 65.35%; H 4.31%; N 5.44%; O 12.44%; S 12.46%

Physical Description: Cryst. (CH₂Cl₂/hexane or Et₂O/hexane)

Melting Point: Mp 78-80° (76-76.5°)

Aldrich: 36663-3

>>Derivative: N-(4-Methylbenzenesulfonyl)

Synonym(s): N-Tosylindole