



>>Entry Name: 5-Indanol, 8Cl

Synonym(s): 2,3-Dihydro-1*H*-inden-5-ol, 9Cl. 5-Hydroxyindane. 5-Hydroxyhydrindene

CAS Registry Number: 1470-94-6

Molecular Formula: C₉H₁₀O

Molecular Weight: 134.177

Accurate Mass: 134.073165

Percentage Composition: C 80.56%; H 7.51%; O 11.92%

Physical Description: Needles (petrol)

Melting Point: Mp 56°

Boiling Point: Bp 225°. Bp₄ 115°

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 3250 mg/kg. LD₅₀ (rbt, skn) 450 mg/kg

Aldrich: I-221-5

Fluka: 56870

>>Derivative: Ac

CAS Registry Number: 5440-82-4

Molecular Formula: C₁₁H₁₂O₂

Molecular Weight: 176.215

Accurate Mass: 176.08373

Percentage Composition: C 74.98%; H 6.86%; O 18.16%

Melting Point: Mp 17-18°

Boiling Point: Bp₁₈ 136°

>>Derivative: Benzoyl

Molecular Formula: C₁₆H₁₄O₂

Molecular Weight: 238.285

Accurate Mass: 238.09938

Percentage Composition: C 80.65%; H 5.92%; O 13.43%

Physical Description: Platelets (EtOH)

Melting Point: Mp 111-112°

>>Derivative: Me ether

Synonym(s): 5-Methoxyindane

CAS Registry Number: 5111-69-3

Molecular Formula: C₁₀H₁₂O

Molecular Weight: 148.204

Accurate Mass: 148.088815

Percentage Composition: C 81.04%; H 8.16%; O 10.80%

Melting Point: Mp 233-234°

Aldrich: 27229-9

>>Derivative: Et ether

Synonym(s): 5-Ethoxyindane

Molecular Formula: C₁₁H₁₄O

Molecular Weight: 162.231

Accurate Mass: 162.104465

Percentage Composition: C 81.44%; H 8.70%; O 9.86%

Boiling Point: Bp 246°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 194C, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1086B, (ir)

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Aldrich Library of FT-NMR Spectra, 1st edn., **2**, 194C, (nmr)

Sadtler Standard C-13 NMR Spectra, 2626, (cmr)

Sadtler Standard Ultraviolet Spectra, 5558, (uv)

Mills, W.H. *et al.*, *J.C.S.*, 1930, 2510, (synth, derivs)

Cook, A.H. *et al.*, *J.C.S.*, 1934, 946, (synth, derivs)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, IBU000