



>>Entry Name: 3-Iodophenol

CAS Registry Number: 626-02-8

Molecular Formula: C₆H₅IO

Molecular Weight: 220.009

Accurate Mass: 219.938513

Percentage Composition: C 32.76%; H 2.29%; I 57.68%; O 7.27%

Physical Description: Needles (petrol)

Melting Point: Mp 40°

pKa Value: pK_a 9.03 (25°)

Other Data: Steam-volatile

Aldrich: I-1000-7

>>Derivative: Benzoyl

Molecular Formula: C₁₃H₉IO₂

Molecular Weight: 324.117

Accurate Mass: 323.964728

Percentage Composition: C 48.17%; H 2.80%; I 39.15%; O 9.87%

Physical Description: Prisms (petrol)

Melting Point: Mp 72-73°

>>Derivative: 4-Methylbenzenesulfonyl

Melting Point: Mp 60-61°

>>Derivative: Me ether

Synonym(s): 1-Iodo-3-methoxybenzene. 3-Iodoanisole

CAS Registry Number: 766-85-8

Molecular Formula: C₇H₇IO

Molecular Weight: 234.036

Accurate Mass: 233.954163

Percentage Composition: C 35.92%; H 3.01%; I 54.22%; O 6.84%

Physical Description: Oil

Boiling Point: Bp 244-245°. Bp₁₄ 123°

Aldrich: 24269-1

>>Derivative: Et ether

Synonym(s): 1-Iodo-3-ethoxybenzene. 3-Iodophenetole

CAS Registry Number: 29052-00-4

Molecular Formula: C₈H₉IO

Molecular Weight: 248.063

Accurate Mass: 247.969813

Percentage Composition: C 38.74%; H 3.66%; I 51.16%; O 6.45%

Physical Description: Oil

Boiling Point: Bp₁₅ 133-134°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 183A, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1042B, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 970B; 1007C, (ir)

Ullmann, F. *et al.*, *Annalen*, 1904, **332**, 66

Buchan, S. *et al.*, *J.C.S.*, 1932, 2857