



>>Entry Name: 4-Iodophenol

CAS Registry Number: 540-38-5

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 (H₂O)

Melting Point: Mp 92-94°

pKa Value: pK_a 9.33 (25°)

Aldrich: I-1020-1

Fluka: 58020

>>Derivative: 4-Methylbenzenesulfonyl

CAS Registry Number: 24962-55-8

Physical Description: Cryst. (MeOH)

Melting Point: Mp 97-99°

>>Derivative: Me ether

Synonym(s): 1-Iodo-4-methoxybenzene. 4-Iodoanisole. Isoform

CAS Registry Number: 696-62-8

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: Needles (MeOH aq.)

Melting Point: Mp 51-52°

Boiling Point: Bp₇₂₆ 237°. Bp₂₅ 139°

Aldrich: I-760-8

Fluka: 57720

>>Derivative: Et ether

Synonym(s): 1-Iodo-4-ethoxybenzene. 4-Iodophenetole

CAS Registry Number: 699-08-1

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: Cryst. (MeOH aq.)

Melting Point: Mp 28-29°

>>Derivative: Trifluoromethyl ether

CAS Registry Number: 103962-05-6

Molecular Formula: C₇H₄F₃IO

Molecular Weight: 288.008

Accurate Mass: 287.925897

Percentage Composition: C 29.19%; H 1.40%; F 19.79%; I 44.06%; O 5.56%

Boiling Point: Bp₁₅ 74-76°

References:

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Baird, W.C. *et al.*, *Prepr.- Am. Chem. Soc., Div. Pet. Chem.*, 1970, **15**, B73, (*synth*)

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