



>>Entry Name: 2,4,6-Triiodophenol, 9CI, 8CI

CAS Registry Number: 609-23-4

Molecular Formula: C₆H₃I₃O

Molecular Weight: 471.803

Accurate Mass: 471.731809

Percentage Composition: C 15.27%; H 0.64%; I 80.69%; O 3.39%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 158-159°

Other Data: Spar. steam-volatile

Hazard & Toxicity: LD₅₀ (rat, orl) 2000 mg/kg

Aldrich: 13772-3

>>Derivative: Ac

Molecular Formula: C₈H₅I₃O₂

Molecular Weight: 513.84

Accurate Mass: 513.742374

Percentage Composition: C 18.70%; H 0.98%; I 74.09%; O 6.23%

Physical Description: Needles or prisms (C₆H₆)

Melting Point: Mp 156°

>>Derivative: Me ether

Synonym(s): 1,3,5-Triiodo-2-methoxybenzene. 2,4,6-Triiodoanisole

Molecular Formula: C₇H₅I₃O

Molecular Weight: 485.829

Accurate Mass: 485.747459

Percentage Composition: C 17.31%; H 1.04%; I 78.36%; O 3.29%

Physical Description: Leaflets (C₆H₆), needles (Et₂O)

Melting Point: Mp 98-99°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1099A, (*ir*)

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Suzuki, H. *et al.*, *Nippon Kagaku Kaishi*, 1963, **84**, 284; *CA*, **58**, 3339, (*synth*)

Lown, J.W. *et al.*, *Can. J. Chem.*, 1977, **55**, 122, (*synth*)

Edgar, K.J. *et al.*, *J.O.C.*, 1990, **55**, 5287, (*synth*, *pmr*, *cmr*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, TKR000