



Type of Compound Code(s): PA2000 PA4700 PA0250 PA0200

Molecular Formula: C₅H₆Cl₂N₂O₂

Molecular Weight: 197.02

Accurate Mass: 195.980632

Percentage Composition: C 30.48%; H 3.07%; Cl 35.99%; N 14.22%; O 16.24%

Use/Importance: Chlorinating agent, disinfectant, used esp. in laundry bleaches. Used as 0.25M soln. in glacial AcOH for potentiometric oxidimetric titration of As(III), Sb(III), Sn(II), Fe(II)

Physical Description: Prisms (CHCl₃)

Melting Point: Mp 132°

Solubility: Sol. H₂O; mod. sol. AcOH, EtOH

Other Data: Liberates HOCl in contact with water

Hazard & Toxicity: Attempted chlorination of xylene caused violent explosion. Severe skin irritant. LD₅₀ (rat, orl) 542 mg/kg. OES: long-term 0.2 mg m⁻³; short-term 0.4 mg m⁻³

Aldrich: 23280-7

Fluka: 35710

>>Derivative: N¹,N³-Dibromo

see 1,3-Dibromo-5,5-dimethyl-2,4-imidazolidinedione, [KHD91-R](#)

>>Derivative: N¹,N³-Diiodo

Synonym(s): 1,3-Diiodo-5,5-dimethyl-2,4-imidazolidinedione. 1,3-Diiodo-5,5-dimethylhydantoin

CAS Registry Number: 2232-12-4

Molecular Formula: C₅H₆I₂N₂O₂

Molecular Weight: 379.924

Accurate Mass: 379.851874

Percentage Composition: C 15.81%; H 1.59%; I 66.81%; N 7.37%; O 8.42%

Use/Importance: Iodinating agent for aromatic compds. and enol acetates

Rare Chemicals Library: S61254-5

>>Derivative: 1-Chloro, 3-bromo

CAS Registry Number: 126-06-7

Molecular Formula: C₅H₆BrClN₂O₂

Molecular Weight: 241.471

Accurate Mass: 239.950116

Percentage Composition: C 24.87%; H 2.50%; Br 33.09%; Cl 14.68%; N 11.60%; O 13.25%

Melting Point: Mp 160-164°

Aldrich: 27711-8

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1315C, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 808A; 808B, (ir)

Slotta, K.H. *et al.*, *Ber.*, 1934, **67**, 1532, (synth)

Bucherer, H.T. *et al.*, *J. Prakt. Chem.*, 1934, **140**, 291; *CA*, **29**, 127, (synth)

Brederek, H. *et al.*, *Annalen*, 1957, **604**, 178, (synth)

Okada, T. *et al.*, *CA*, 1957, **51**, 13852, (synth)

Kamennov, N.A. *et al.*, *CA*, 1967, **67**, 90725, (synth)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 259; **3**, 4; **7**, 126

U.S. Pat., 1973, 3 752 821; *CA*, **79**, 92221, (synth)

Merck Index, 10th edn., 1983, No. 3049, (Dactin)

Radhamma, M.P. *et al.*, *Talanta*, 1983, **30**, 49, (use)

Schläpfer-Däler, M. *et al.*, *Helv. Chim. Acta*, 1992, **75**, 1251, (1-Me)

Fujisaki, S. *et al.*, *Bull. Chem. Soc. Jpn.*, 1993, **66**, 2426, (dibromo)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BNA325; DFE200; DSF300

Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworths, 1990, 1748