



>>Entry Name: 1,1,1,3,3,3-Hexachloro-2-propanone, 9Cl

Synonym(s): Hexachloroacetone. HCA, WSSA

CAS Registry Number: 116-16-5

Cl3CCOCCl3

Molecular Formula: C₃Cl₆O

Molecular Weight: 264.749

Accurate Mass: 261.808027

Percentage Composition: C 13.61%; Cl 80.35%; O 6.04%

Biological Source: Constit. of *Osmanthus fragrans*. Isol from the alga *Asparagopsis taxiformis*

Use/Importance: Source of positive chlorine in enamine reactions. Herbicide, now superseded

Physical Description: Liq.

Melting Point: Fp -2°

Boiling Point: Bp 202-204°. Bp₂₆ 99-101.5°

Solubility: Sl. sol. H₂O

Density: d₄¹² 1.74

Hazard & Toxicity: LD₅₀ (rat, orl) 1290 mg/kg; LD₅₀ (rat, skn) 2980 mg/kg

Aldrich: H530-8

Fluka: 52080

Sigma: H6887

>>Derivative: Tetrahydrate

Physical Description: Unstable cryst.

Melting Point: Mp 39.5-40.5° (incongruent)

Other Data: Unstable. Previously thought to be a covalent monohydrate

References:

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Andersen, P. *et al.*, *Acta Chem. Scand., Ser. A*, 1974, **28**, 239, (struct)

Hawkes, G.E. *et al.*, *J.O.C.*, 1974, **39**, 1276, (cmr)

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