



>>Entry Name: (2,2,2-Trichloro-1-hydroxyethyl)carbamic acid, 9CI

Cl3CCH(OH)NHCOOH

Molecular Formula: C₃H₄Cl₃NO₃

Molecular Weight: 208.428

Accurate Mass: 206.925675

Percentage Composition: C 17.29%; H 1.93%; Cl 51.03%; N 6.72%; O 23.03%

>>Derivative: Et ester

Synonym(s): Ethyl trichloramate. **Carbocloral**, BAN, INN, USAN. Chloral urethane. Prodorm. Tradal. Ural. Uraline. CI 336. CN 16146. Hy 185. NSC 33077

CAS Registry Number: 541-79-7

Molecular Formula: C₅H₈Cl₃NO₃

Molecular Weight: 236.481

Accurate Mass: 234.956975

Percentage Composition: C 25.40%; H 3.41%; Cl 44.98%; N 5.92%; O 20.30%

Use/Importance: Hypnotic, anticonvulsant agent

Development Status: Never marketed

Melting Point: Mp 103 part dec.°

Solubility: Spar. sol. H₂O (1 g per 100 cm³ at 25°)

Calculated Log P Data: Log P 1.91 (calc)

Hazard & Toxicity: LD_{Lo} (rat, orl) 1500 mg/kg

Rare Chemicals Library: S16980-3

>>Derivative: Benzyl ester

CAS Registry Number: 6798-34-1

Molecular Formula: C₁₀H₁₀Cl₃NO₃

Molecular Weight: 298.552

Accurate Mass: 296.972625

Percentage Composition: C 40.23%; H 3.38%; Cl 35.62%; N 4.69%; O 16.08%

Physical Description: Cryst. (C₆H₆/toluene)

Melting Point: Mp 114-115°

Rare Chemicals Library: S7116-2

References:

Bischoff, C., *Ber.*, 1874, **7**, 628, (*carbocloral*)

Glazko, A.J. *et al.*, *J. Pharmacol. Exp. Ther.*, 1957, **121**, 119-129; 136-143, (*props, metab, pharmacol*)

Weygand, F. *et al.*, *Chem. Ber.*, 1966, **99**, 1944-1956, (*ester*)

Belaissaoui, A. *et al.*, *Can. J. Chem.*, 1997, **75**, 523-530, (*Et ester, synth, ir, pmr, cmr*)