



>>Entry Name: Triclofos, BAN, INN

Synonym(s): 2,2,2-Trichloroethanol dihydrogen phosphate, 9Cl, 8Cl. Mono(2,2,2-trichloroethyl) phosphate

CAS Registry Number: 306-52-5



Molecular Formula: $\text{C}_2\text{H}_4\text{Cl}_3\text{O}_4\text{P}$

Molecular Weight: 229.383

Accurate Mass: 227.891278

Percentage Composition: C 10.47%; H 1.76%; Cl 46.37%; O 27.90%; P 13.50%

Use/Importance: Sedative, hypnotic

Physical Description: Cryst. (C_6H_6)

Melting Point: Mp 120-121°

>>Derivative: Mono-Na salt

Synonym(s): Triclofos sodium, USAN. Triclos. Tricloryl. Hipnogal. Sch 10159. Tricleryl. Tricloran

CAS Registry Number: 7246-20-0

>>Derivative: Monoanilinium salt

Physical Description: Solid

Melting Point: Mp 116-118°

>>Derivative: Monocyclohexylammonium salt

Physical Description: Solid

Melting Point: Mp 139-140°

>>Derivative: Dichloride

Synonym(s): 2,2,2-Trichloroethyl phosphorodichloridate. 2,2,2-Trichloroethyl phosphoryl dichloride

CAS Registry Number: 18868-46-7

Molecular Formula: $\text{C}_2\text{H}_2\text{Cl}_5\text{O}_2\text{P}$

Molecular Weight: 266.274

Accurate Mass: 263.823502

Percentage Composition: C 9.02%; H 0.76%; Cl 66.57%; O 12.02%; P 11.63%

Use/Importance: Precursor to reagents employed in nucleotide and phospholipid synth.

Physical Description: Liq.

Boiling Point: Bp₁₄ 116-118°

Aldrich: 24216-0

Sigma: T5892

References:

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **1**, 1499B, (*nmr*)

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Gerrard, W. *et al.*, *J.C.S.*, 1954, 1148, (*dichloride*)

Hems, B.A. *et al.*, *Br. Med. J.*, 1962, **1**, 1834, (*synth*)

Murakami, Y. *et al.*, *J.C.S. Perkin 2*, 1973, 1235, (*ir, props*)

Owen, G.R. *et al.*, *Synthesis*, 1974, 704, (*synth, dichloride, ir*)

Lammers, J.G. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1977, **96**, 216, (*use*)

Gajda, T. *et al.*, *Synthesis*, 1977, 623, (*synth*)

Sellers, E.M. *et al.*, *J. Clin. Pharmacol.*, 1978, **18**, 457, (*metab*)

Markowska, A. *et al.*, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1979, **27**, 115, (*synth*)

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