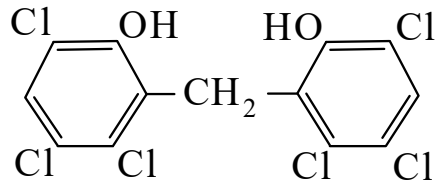
>>**Entry Name: 2,2',3,3',5,5'-Hexachloro-6,6'-dihydroxydiphenylmethane**
Synonym(s): 2,2'-Methylenebis[3,4,6-trichlorophenol], 9CI, 8CI. Hexachlorophane, BAN. **Hexachlorophene,** INN**.** Anacal. Derl. Dermalex. Gramophen. Phisohex. Torbetol. AT 7. Many other names



CAS Registry Number: 70-30-4

Molecular Formula: $C_{13}H_6Cl_6O_2$
Molecular Weight: 406.905
Accurate Mass: 403.849892
Percentage Composition: C 38.37%; H 1.49%; Cl 52.28%; O 7.86%
Use/Importance: Skin disinfectant, anthelmintic (veterinary). Pharmacol. tool for inducing brain damage (cytotoxic brain oedema)
Melting Point: Mp 164-165°
Calculated Log P Data: Log P 7.08 (uncertain value) (calc)
Hazard & Toxicity: Dermal absorption has caused spongiform encephalopathy in infants. Prolonged use can cause hypersensitivity reactions incl. photosensitisation. LD_{50} (rat, orl) 56 mg/kg. LD_{50} (rat, skn) 1840 mg/kg. Causes brain lesions exp.

Aldrich: 30711-4
Sigma: H4625
Supelco: 44-2610

>>**Derivative:** Monophosphate
Synonym(s): Hexachlorophene monophosphate. Hepadist. Ph 1503

CAS Registry Number: 3046-99-9
Molecular Formula: $C_{13}H_7Cl_6O_5P$
Molecular Weight: 486.885
Accurate Mass: 483.816224
Percentage Composition: C 32.07%; H 1.45%; Cl 43.69%; O 16.43%; P 6.36%

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 325C, *(nmr)*
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1120B, *(ir)*
U.K. Pat., 1956, *ICI*, 760 342; *CA*, **51**, 12140i, *(synth)*
U.S. Pat., 1957, *Givaudan*, 2 812 365; *CA*, **52**, 5473
Sammul, O.R. *et al.*, *J. Assoc. Off. Agric. Chem.*, 1964, **47**, 918, *(ir)*
Netherlands Pat., 1965, 283 922; *CA*, **63**, 9869, *(deriv)*
Dietrich, M.W. *et al.*, *J. Am. Oil Chem. Soc.*, 1967, **44**, 491, *(nmr)*
Czech. Pat., 1969, 134 656; *CA*, **75**, 5481r, *(synth)*
Kimbrough, R.*, Clin. Toxicol.*, 1976, **9**, 969, *(pharmacol, tox)*
IARC Monog., 1979, **20**, 241; *Suppl*. 7, 64, *(rev, tox)*
Freundt, K.J. *et al.*, *Dtsch. Apoth. -Ztg.*, 1983, **123**, 41, *(rev)*
Negwer, M.*, Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 2615, *(synonyms)*
Purves, D.C. *et al.*, *Human Exp. Toxicol.*, 1991, **10**, 439, *(tox)*
Andreas, K.*, Naunyn-Schmiedeberg's Arch. Pharmacol.*, 1993, **347**, 79, *(pharmacol, tox)*
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1133
Lewis, R.J.*, Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HCL000

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