Phosphoric acid, tris(p-chlorophenyl) ester

Other names:	Tris(4-chlorophenyl) phosphate
Inchi:	InChI=1S/C18H12Cl3O4P/c19-13-1-7-16(8-2-13)23-26(22,24-17-9-3-14(20)4-10-17)25-1
InchiKey:	DFQHFXCKNSCDFW-UHFFFAOYSA-N
Formula:	C18H12Cl3O4P
SMILES:	O=P(Oc1ccc(Cl)cc1)(Oc1ccc(Cl)cc1)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	429.62
CAS:	3871-31-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.19		Crippen Method
logp	7.292		Crippen Method
mcvol	273.860	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3871316&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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