

O,O-Dimethyl O-(2,4,5-trichloro)phenyl phosphate

Other names:	Phosphoric acid, dimethyl 2,4,5-trichlorophenyl ester Dimethyl (2,4,5-trichlorophenyl) phosphate Dowco 101 Fenchlorphos-oxon Ronnell oxon Ronnell oxygen analog Ronnoxon Ronoxon Fenchlorophos oxygen analog NSC 133018
Inchi:	InChI=1S/C8H8Cl3O4P/c1-13-16(12,14-2)15-8-4-6(10)5(9)3-7(8)11/h3-4H,1-2H3
InchiKey:	XWMMHXRGYYPFAV-UHFFFAOYSA-N
Formula:	C8H8Cl3O4P
SMILES:	COP(=O)(OC)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	305.48
CAS:	3983-45-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.50		Crippen Method
logp	4.426		Crippen Method
mcvol	180.480	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3983457&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemed.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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