O-(4-methylphenyl) dichloridothiophosphate

Inchi: InChI=1S/C7H7Cl2OPS/c1-6-2-4-7(5-3-6)10-11(8,9)12/h2-5H,1H3
InchiKey: RDGYPSHBQMWDHX-UHFFFAOYSA-N
Formula: C7H7Cl2OPS
SMILES: Cc1ccc(OP(=S)(Cl)Cl)cc1
Mol. weight [g/mol]: 241.07
CAS: 18961-95-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.21		Crippen Method
logp	4.076		Crippen Method
mcvol	152.890	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18961950&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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