O-(4-tert-butylphenyl) 0-phenyl phosphorochloridate

Inchi: InChI=1S/C16H18ClO3P/c1-16(2,3)13-9-11-15(12-10-13)20-21(17,18)19-14-7-5-4-6-8-14

InchiKey: KOXGHOLJUDEKOQ-UHFFFAOYSA-N

Formula: C16H18ClO3P

SMILES: CC(C)(C)c1ccc(OP(=O)(Cl)Oc2ccccc2)cc1

Mol. weight [g/mol]: 324.74

CAS: 63449-81-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.25		Crippen Method
logp	5.789		Crippen Method
mcvol	239.090	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C63449810&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume