

O-(4-tert-butylphenyl) O-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/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/74-033-3/O-4-tert-butylphenyl-O-phenyl-phosphorochloridate.pdf>

Generated by Cheméo on 2024-04-25 19:38:55.85054886 +0000 UTC m=+16363184.771126175.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.