4-([Bis(4-tert-butylphenoxy)phosphoryl]oxy)-1,1'-l

Inchi:	InChI=1S/C32H35O4P/c1-31(2,3)26-14-20-29(21-15-26)35-37(33,36-30-22-16-27(17-23-
InchiKey:	XIMHJOXJJAWQOT-UHFFFAOYSA-N
Formula:	C32H35O4P
SMILES:	CC(C)(C)c1ccc(OP(=O)(Oc2ccc(-c3ccccc3)cc2)Oc2ccc(C(C)(C)C)cc2)cc1
Mol. weight [g/mol]:	514.59
CAS:	116401-97-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.37		Crippen Method
logp	9.593		Crippen Method
mcvol	410.640	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401979&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

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