

[1,1'-Biphenyl]-2-yl 4-tert-butylphenyl phenyl phosphate

Inchi:	InChI=1S/C28H27O4P/c1-28(2,3)23-18-20-25(21-19-23)31-33(29,30-24-14-8-5-9-15-24)
InchiKey:	FJYBMEAYPNNHJG-UHFFFAOYSA-N
Formula:	C28H27O4P
SMILES:	CC(C)(C)c1ccc(OP(=O)(Oc2ccccc2)Oc2ccccc2-c2ccccc2)cc1
Mol. weight [g/mol]:	458.49
CAS:	116401-98-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.05		Crippen Method
logp	8.296		Crippen Method
mcvol	354.280	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401980&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

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