

Di[1,1'-biphenyl]-2-yl 4-cyclohexylphenyl phosphate

Inchi:	InChI=1S/C36H33O4P/c37-41(38-32-26-24-29(25-27-32)28-14-4-1-5-15-28,39-35-22-12
InchiKey:	SQZKSNXTNMWAAB-UHFFFAOYSA-N
Formula:	C36H33O4P
SMILES:	O=P(Oc1ccc(C2CCCCC2)cc1)(Oc1cccc1-c1cccc1)Oc1cccc1-c1cccc1
Mol. weight [g/mol]:	560.62
CAS:	116402-01-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.68		Crippen Method
logp	10.713		Crippen Method
mcvol	432.380	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=C116402018&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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