Di[1,1'-biphenyl]-3-yl phenyl phosphate

Inchi: InChI=1S/C30H23O4P/c31-35(32-28-18-8-3-9-19-28,33-29-20-10-16-26(22-29)24-12-4-1
InchiKey: QCWIDHPPOSNLLN-UHFFFAOYSA-N
Formula: C30H23O4P
SMILES: O=P(Oc1ccccc1)(Oc1cccc(-c2ccccc2)c1)Oc1cccc(-c2ccccc2)c1
Mol. weight [g/mol]: 478.48
CAS: 116402-03-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.34		Crippen Method
logp	8.665		Crippen Method
mcvol	358.700	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402030&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume