Bis(4-tert-butylphenyl) phenyl phosphate

Inchi: InChI=1S/C26H31O4P/c1-25(2,3)20-12-16-23(17-13-20)29-31(27,28-22-10-8-7-9-11-22)
InchiKey: PDLPMCXGPIVYQQ-UHFFFAOYSA-N
Formula: C26H31O4P
SMILES: CC(C)(C)c1ccc(OP(=O)(Oc2ccccc2)Oc2ccc(C(C)(C)C)cc2)cc1
Mol. weight [g/mol]: 438.50
CAS: 115-87-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.76		Crippen Method
logp	7.927		Crippen Method
mcvol	349.860	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=C115877&Units=SI

Legend

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