Bis(4-tert-butyl-2-methylphenyl) phenyl phosphate

Inchi: InChI=1S/C28H35O4P/c1-20-18-22(27(3,4)5)14-16-25(20)31-33(29,30-24-12-10-9-11-13

InchiKey: SKPHTQCQZCURIC-UHFFFAOYSA-N

Formula: C28H35O4P

SMILES: Cc1cc(C(C)(C)C)ccc1OP(=O)(Oc1ccccc1)Oc1ccc(C(C)(C)C)cc1C

Mol. weight [g/mol]: 466.55

CAS: 116402-04-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.72		Crippen Method
logp	8.543		Crippen Method
mcvol	378.040	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402041&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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