

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

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=C116402041&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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