Phenol, 4-(1,1-dimethylethyl)-, phosphate (3:1)

Other names:	p-tert-Butylphenol, phosphate (3:1)
	Phenol, p-tert-butyl-, phosphate (3:1)
	Tris(p-tert-butylphenyl) phosphate
	Tris(4-tert-butylphenyl) phosphate
Inchi:	InChI=1S/C30H39O4P/c1-28(2,3)22-10-16-25(17-11-22)32-35(31,33-26-18-12-23(13-19-
InchiKey:	LORSVOJSXMHDHF-UHFFFAOYSA-N
Formula:	C30H39O4P
SMILES:	CC(C)(C)c1ccc(OP(=O)(Oc2ccc(C(C)(C)C)cc2)Oc2ccc(C(C)(C)C)cc2)cc1
Mol. weight [g/mol]:	494.60
CAS:	78-33-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.08		Crippen Method
logp	9.224		Crippen Method
mcvol	406.220	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78331&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

Latest version available from: