

P-sec-butyl phenyl phosphate

Inchi:	InChI=1S/C30H39O4P/c1-7-22(4)25-10-16-28(17-11-25)32-35(31,33-29-18-12-26(13-19
InchiKey:	CVQJIHIPOBDGET-UHFFFAOYSA-N
Formula:	C30H39O4P
SMILES:	CCC(C)c1ccc(OP(=O)(Oc2ccc(C(C)CC)cc2)Oc2ccc(C(C)CC)cc2)cc1
Mol. weight [g/mol]:	494.60
CAS:	116402-16-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.95		Crippen Method
logp	9.872		Crippen Method
mcvol	406.220	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402165&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/97-185-0/P-sec-butyl-phenyl-phosphate.pdf>

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