Dibutyl 4-methyl-phenyl phosphate

Inchi: InChI=1S/C15H25O4P/c1-4-6-12-17-20(16,18-13-7-5-2)19-15-10-8-14(3)9-11-15/h8-11H
InchiKey: AXVQGNPTHCNQLJ-UHFFFAOYSA-N
Formula: C15H25O4P
SMILES: CCCCOP(=O)(OCCCC)Oc1ccc(C)cc1
Mol. weight [g/mol]: 300.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.44		Crippen Method
logp	5.115		Crippen Method
mcvol	242.390	ml/mol	McGowan Method
rinpol	2047.00		NIST Webbook
rinpol	2047.00		NIST Webbook
ripol	2630.00		NIST Webbook
ripol	2630.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R168895&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
rinpol: Non-polar retention indices
ripol: Polar retention indices