Dibutyl 4-bromo-phenyl phosphate

Inchi: InChI=1S/C14H22BrO4P/c1-3-5-11-17-20(16,18-12-6-4-2)19-14-9-7-13(15)8-10-14/h7-1
InchiKey: SYGNAIVBBLSRJL-UHFFFAOYSA-N
Formula: C14H22BrO4P
SMILES: CCCCOP(=O)(OCCCC)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 365.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	5.569		Crippen Method
mcvol	245.800	ml/mol	McGowan Method
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
ripol	2810.00		NIST Webbook
ripol	2810.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R168855&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
rinpol: Non-polar retention indices
ripol: Polar retention indices