Phenylphosphonic acid, hexyl isobutyl ester

Inchi: InChI=1S/C16H27O3P/c1-4-5-6-10-13-18-20(17,19-14-15(2)3)16-11-8-7-9-12-16/h7-9,11
InchiKey: QRIQDVSPMSEZGW-UHFFFAOYSA-N
Formula: C16H27O3P
SMILES: CCCCCCOP(=O)(OCC(C)C)c1ccccc1
Mol. weight [g/mol]: 298.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.22		Crippen Method
logp	4.774		Crippen Method
mcvol	250.610	ml/mol	McGowan Method
rinpol	2034.00		NIST Webbook
rinpol	2034.00		NIST Webbook

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=U393217&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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