Bis(2-methylbutyl) hydrogen phosphite

Inchi: InChI=1S/C10H23O3P/c1-5-9(3)7-12-14(11)13-8-10(4)6-2/h9-10,14H,5-8H2,1-4H3
InchiKey: IILGBAUIRAQOMD-UHFFFAOYSA-N
Formula: C10H23O3P
SMILES: CCC(C)CO[PH](=O)OCC(C)CC
Mol. weight [g/mol]: 222.26
CAS: 62317-12-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.16		Crippen Method
logp	3.502		Crippen Method
mcvol	189.830	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=C62317128&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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