Phosphorous acid, bis(2,2-dimethylpentyl) ester

Inchi: InChI=1S/C14H31O3P/c1-7-9-13(3,4)11-16-18(15)17-12-14(5,6)10-8-2/h18H,7-12H2,1-6

InchiKey: FFDNQLLGYMRACP-UHFFFAOYSA-N

Formula: C14H31O3P

SMILES: CCCC(C)(C)CO[PH](=O)OCC(C)(C)CCC

Mol. weight [g/mol]: 278.37

CAS: 116402-21-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.84		Crippen Method
logp	5.062		Crippen Method
mcvol	246.190	ml/mol	McGowan Method

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=C116402212&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