Methylphosphonic acid, methyl-(4-methyl-2-pentyl) ester

Inchi: InChI=1S/C8H19O3P/c1-7(2)6-8(3)11-12(5,9)10-4/h7-8H,6H2,1-5H3
InchiKey: UUWSXHSBLUIENO-UHFFFAOYSA-N
Formula: C8H19O3P
SMILES: COP(C)(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 194.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	2.907		Crippen Method
mcvol	161.650	ml/mol	McGowan Method
rinpol	755.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R548479&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