Phosphonic acid, methyl-, dipentyl ester

Other names:	Methylphosphonic acid, dipentyl ester
	Diamyl methylphosphonate
	Dipentyl methylphosphonate
Inchi:	InChI=1S/C11H25O3P/c1-4-6-8-10-13-15(3,12)14-11-9-7-5-2/h4-11H2,1-3H3
InchiKey:	IYWHBXSPNUEWOS-UHFFFAOYSA-N
Formula:	C11H25O3P
SMILES:	CCCCCOP(C)(=O)OCCCCC
Mol. weight [g/mol]:	236.29
CAS:	1000-36-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.88		Crippen Method
logp	4.223		Crippen Method
mcvol	203.920	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1000368&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