

Phosphonic acid, methyl-, o,o-diisopentyl ester

Other names:	Diisopentyl methylphosphonate Methylphosphonic acid di-(3-methylbutyl) ester
Inchi:	InChI=1S/C11H25O3P/c1-10(2)6-8-13-15(5,12)14-9-7-11(3)4/h10-11H,6-9H2,1-5H3
InchiKey:	YXHUEGLTOGMNPE-UHFFFAOYSA-N
Formula:	C11H25O3P
SMILES:	CC(C)CCOP(C)(=O)OCCC(C)C
Mol. weight [g/mol]:	236.29
CAS:	2452-70-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.39		Crippen Method
logp	3.935		Crippen Method
mcvol	203.920	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2452702&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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