

Methylphosphonic acid, isobutyl pinacolyl ester

Inchi:	InChI=1S/C11H25O3P/c1-9(2)8-13-15(7,12)14-10(3)11(4,5)6/h9-10H,8H2,1-7H3
InchiKey:	NVIZGQRWMJYKRE-UHFFFAOYSA-N
Formula:	C11H25O3P
SMILES:	CC(C)COP(C)(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]:	236.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.50		Crippen Method
logp	3.933		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.cheméo.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=R334879&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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