

Methylphosphonic acid, methyl-(3-methylbutyl) ester

Other names:	Methylphosphonic acid, 3-methyl-1-butyl, methyl ester
Inchi:	InChI=1S/C7H17O3P/c1-7(2)5-6-10-11(4,8)9-3/h7H,5-6H2,1-4H3
InchiKey:	QCVGEMUTTZNUGZ-UHFFFAOYSA-N
Formula:	C7H17O3P
SMILES:	COP(C)(=O)OCCC(C)C
Mol. weight [g/mol]:	180.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.96		Crippen Method
logp	2.518		Crippen Method
mcvol	147.560	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=R548464&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

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