

Methylphosphonic acid, isobutyl isopropyl ester

Inchi:	InChI=1S/C8H19O3P/c1-7(2)6-10-12(5,9)11-8(3)4/h7-8H,6H2,1-5H3
InchiKey:	UPZJYWUMMFKOGJ-UHFFFAOYSA-N
Formula:	C8H19O3P
SMILES:	CC(C)COP(C)(=O)OC(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
rinsol	1142.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R403693&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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<https://www.chemeo.com/cid/69-015-9/Methylphosphonic-acid-isobutyl-isopropyl-ester.pdf>

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