

# Phosphonic acid, (1-carbamoylethyl)-, diethyl ester

Inchi:	InChI=1S/C7H16NO4P/c1-4-11-13(10,12-5-2)6(3)7(8)9/h6H,4-5H2,1-3H3,(H2,8,9)
InchiKey:	OSGRVDNHAGXYME-UHFFFAOYSA-N
Formula:	C7H16NO4P
SMILES:	CCOP(=O)(OCC)C(C)C(N)=O
Mol. weight [g/mol]:	209.18
CAS:	52111-19-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	1.126		Crippen Method
mcvol	159.110	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C52111190&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C52111190&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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