

# Triethyl 3-phosphonopropanoate

<b>Other names:</b>	Triethyl 3-phosphonopropionate 3-Diethylphosphonopropionic acid ethyl ester Propanoic acid, 3-(diethoxyphosphinyl)-, ethyl ester Propionic acid, 3-diethoxy phosphinyl, ethyl ester Ethyl 3-(diethylphosphono)propanoate
<b>Inchi:</b>	InChI=1S/C9H19O5P/c1-4-12-9(10)7-8-15(11,13-5-2)14-6-3/h4-8H2,1-3H3
<b>InchiKey:</b>	JMJWCUOIOKBVNQ-UHFFFAOYSA-N
<b>Formula:</b>	C9H19O5P
<b>SMILES:</b>	CCOC(=O)CCP(=O)(OCC)OCC
<b>Mol. weight [g/mol]:</b>	238.22
<b>CAS:</b>	3699-67-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.90		Crippen Method
logp	2.206		Crippen Method
mcvol	183.180	ml/mol	McGowan Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3699670&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3699670&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

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