

# diethyl (4-methylbenzyl)phosphonate

<b>Inchi:</b>	InChI=1S/C12H19O3P/c1-4-14-16(13,15-5-2)10-12-8-6-11(3)7-9-12/h6-9H,4-5,10H2,1-3
<b>InchiKey:</b>	QKGBKPZAXXBLJE-UHFFFAOYSA-N
<b>Formula:</b>	C12H19O3P
<b>SMILES:</b>	CCOP(=O)(Cc1ccc(C)cc1)OCC
<b>Mol. weight [g/mol]:</b>	242.25
<b>CAS:</b>	3762-25-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.95		Crippen Method
logp	3.761		Crippen Method
mcvol	194.250	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=C3762252&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3762252&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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