

Phosphonic acid, ethyl-, dimethyl ester

Other names:	Ethylphosphonic acid, dimethyl ester Dimethyl ethylphosphonate Ethylphosphonic acid, Me
Inchi:	InChI=1S/C4H11O3P/c1-4-8(5,6-2)7-3/h4H2,1-3H3
InchiKey:	YHQMSHVVGOSZEW-UHFFFAOYSA-N
Formula:	C4H11O3P
SMILES:	CCP(=O)(OC)OC
Mol. weight [g/mol]:	138.10
CAS:	6163-75-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.95		Crippen Method
logp	1.492		Crippen Method
mcvol	105.290	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6163753&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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<https://www.chemeo.com/cid/96-707-1/Phosphonic-acid-ethyl-dimethyl-ester.pdf>

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