

Ethyl methyl methylphosphonate

Other names:	Methyl-phosphonic acid ethyl ester methyl ester
Inchi:	InChI=1S/C4H11O3P/c1-4-7-8(3,5)6-2/h4H2,1-3H3
InchiKey:	YDVMILOIKRSPEO-UHFFFAOYSA-N
Formula:	C4H11O3P
SMILES:	CCOP(C)(=O)OC
Mol. weight [g/mol]:	138.10
CAS:	18755-36-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.95		Crippen Method
logp	1.492		Crippen Method
mcvol	105.290	ml/mol	McGowan Method
rinpol	952.00		NIST Webbook
rinpol	951.50		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	952.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18755367&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices

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