

Phosphonic acid, methyl, cyclopentyl methyl ester

Other names:	Methylphosphonic acid, methyl cyclopentyl ester Methyl cyclopentyl methylphosphonate Methylphosphonic acid, cyclopentyl, methyl ester
Inchi:	InChI=1S/C7H15O3P/c1-9-11(2,8)10-7-5-3-4-6-7/h7H,3-6H2,1-2H3
InchiKey:	CEYXBFDPWJSKHZ-UHFFFAOYSA-N
Formula:	C7H15O3P
SMILES:	COP(C)(=O)OC1CCCC1
Mol. weight [g/mol]:	178.17
CAS:	88053-17-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.21		Crippen Method
logp	2.415		Crippen Method
mcvol	136.700	ml/mol	McGowan Method
rinpol	825.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	825.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88053172&Units=SI

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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