

Dipropyl methylphosphonate

Other names:	Methylphosphonic acid, dipropyl ester
Inchi:	InChI=1S/C7H17O3P/c1-4-6-9-11(3,8)10-7-5-2/h4-7H2,1-3H3
InchiKey:	NRMHUSQXOMWJGD-UHFFFAOYSA-N
Formula:	C7H17O3P
SMILES:	CCCOP(C)(=O)OCCC
Mol. weight [g/mol]:	180.18
CAS:	6410-56-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.20		Crippen Method
logp	2.663		Crippen Method
mcvol	147.560	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=C6410566&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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