

Dibutyl methanephosphonate

Other names:	DBMP Dibutyl methylphosphonate Phosphonic acid, methyl-, dibutyl ester Phosphonic acid, methyl-, O,O-dibutyl ester Methylphosphonic acid, dibutyl ester
Inchi:	InChI=1S/C9H21O3P/c1-4-6-8-11-13(3,10)12-9-7-5-2/h4-9H2,1-3H3
InchiKey:	NPNBLTJGRBYCJB-UHFFFAOYSA-N
Formula:	C9H21O3P
SMILES:	CCCCOP(C)(=O)OCCCC
Mol. weight [g/mol]:	208.24
CAS:	2404-73-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.04		Crippen Method
logp	3.443		Crippen Method
mcvol	175.740	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=C2404731&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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