

dimethyl hydrogen phosphate

Inchi:	InChI=1S/C2H7O4P/c1-5-7(3,4)6-2/h1-2H3,(H,3,4)
InchiKey:	KKUKTXOBAAWVSHC-UHFFFAOYSA-N
Formula:	C2H7O4P
SMILES:	COP(=O)(O)OC
Mol. weight [g/mol]:	126.05
CAS:	813-78-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.36		Crippen Method
logp	0.380		Crippen Method
mcvol	82.980	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=C813785&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

Latest version available from:

<https://www.chemeo.com/cid/100-490-6/dimethyl-hydrogen-phosphate.pdf>

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