

Propionic acid, 3-diethyl-phosphono-, methyl ester

Inchi:	InChI=1S/C8H17O5P/c1-4-12-14(10,13-5-2)7-6-8(9)11-3/h4-7H2,1-3H3
InchiKey:	TXMSAFGVEZUMPX-UHFFFAOYSA-N
Formula:	C8H17O5P
SMILES:	CCOP(=O)(CCC(=O)OC)OCC
Mol. weight [g/mol]:	224.19
CAS:	1112-94-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Crippen Method
logp	1.816		Crippen Method
mcvol	169.090	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C1112943&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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