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/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=C1112943&Units=SI

Legend

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