

Valeric acid, 2-(diethylphosphono), methyl ester

Inchi:	InChI=1S/C10H21O5P/c1-5-8-9(10(11)13-4)16(12,14-6-2)15-7-3/h9H,5-8H2,1-4H3
InchiKey:	WBYUTIJGRBZOGJ-UHFFFAOYSA-N
Formula:	C10H21O5P
SMILES:	CCCC(C(=O)OC)P(=O)(OCC)OCC
Mol. weight [g/mol]:	252.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	2.594		Crippen Method
mcvol	197.270	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=B6008247&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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