

Propionic acid, 3-(diethylphosphono)-2,2-dimethylethyl ester

Other names:	Pivalic acid, diethylphosphono-, ethyl ester
Inchi:	InChI=1S/C11H23O5P/c1-6-14-10(12)11(4,5)9-17(13,15-7-2)16-8-3/h6-9H2,1-5H3
InchiKey:	UTHLSHQUNFTYKP-UHFFFAOYSA-N
Formula:	C11H23O5P
SMILES:	CCOC(=O)C(C)(C)CP(=O)(OCC)OCC
Mol. weight [g/mol]:	266.27
CAS:	116594-67-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.50		Crippen Method
logp	2.842		Crippen Method
mcvol	211.360	ml/mol	McGowan Method

Sources

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=C116594673&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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