

Propionic acid, 2-diethylphosphono-2-hydroxy-, ethyl ester

Inchi:	InChI=1S/C9H19O6P/c1-5-13-8(10)9(4,11)16(12,14-6-2)15-7-3/h11H,5-7H2,1-4H3
InchiKey:	JLLYCECFPBUIFU-UHFFFAOYSA-N
Formula:	C9H19O6P
SMILES:	CCOC(=O)C(C)(O)P(=O)(OCC)OCC
Mol. weight [g/mol]:	254.22
CAS:	20824-52-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.77		Crippen Method
logp	1.524		Crippen Method
mcvol	189.050	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C20824526&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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