

Propionic acid, 2-(diisopropylphosphono)-, methyl ester

Inchi:	InChI=1S/C10H21O5P/c1-7(2)14-16(12,15-8(3)4)9(5)10(11)13-6/h7-9H,1-6H3
InchiKey:	VYFHWHULKKBRCX-UHFFFAOYSA-N
Formula:	C10H21O5P
SMILES:	COC(=O)C(C)P(=O)(OC(C)C)OC(C)C
Mol. weight [g/mol]:	252.24
CAS:	31460-07-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.65		Crippen Method
logp	2.591		Crippen Method
mcvol	197.270	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=C31460078&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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