Mono-di-iso-propyl acid o-phosphate

Other names:	diisopropyl hydrogen phosphate
Inchi:	InChI=1S/C6H15O4P/c1-5(2)9-11(7,8)10-6(3)4/h5-6H,1-4H3,(H,7,8)
InchiKey:	WZPMZMCZAGFKOC-UHFFFAOYSA-N
Formula:	C6H15O4P
SMILES:	CC(C)OP(=O)(O)OC(C)C
Mol. weight [g/mol]:	182.15
CAS:	1611-31-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	1.937		Crippen Method
mcvol	139.340	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=C1611310&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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