Acetic acid, phosphono-, p,p-diisopropyl c-benzyl ester

Inchi:	InChI=1S/C15H23O5P/c1-12(2)19-21(17,20-13(3)4)11-15(16)18-10-14-8-6-5-7-9-14/h5-9
InchiKey:	VDDRVGUAAAIRIO-UHFFFAOYSA-N
Formula:	C15H23O5P
SMILES:	CC(C)OP(=O)(CC(=O)OCc1ccccc1)OC(C)C
Mol. weight [g/mol]:	314.31
CAS:	109643-29-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.23		Crippen Method
logp	3.773		Crippen Method
mcvol	243.960	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109643290&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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