

Isobutyric acid, 3-diisobutoxy-phosphinyl-, methyl ester

Inchi:	InChI=1S/C13H27O5P/c1-10(2)7-17-19(15,18-8-11(3)4)9-12(5)13(14)16-6/h10-12H,7-9H
InchiKey:	QZZBQOSHOLMNCH-UHFFFAOYSA-N
Formula:	C13H27O5P
SMILES:	COC(=O)C(C)CP(=O)(OCC(C)C)OCC(C)C
Mol. weight [g/mol]:	294.32
CAS:	116595-32-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	3.334		Crippen Method
mcvol	239.540	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116595325&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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