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