

Phosphonic acid, methyl-, o,o-bis-(3,3-dimethyl butyl) ester

Inchi:	InChI=1S/C13H29O3P/c1-12(2,3)8-10-15-17(7,14)16-11-9-13(4,5)6/h8-11H2,1-7H3
InchiKey:	IKQCEQDGORUWEV-UHFFFAOYSA-N
Formula:	C13H29O3P
SMILES:	CC(C)(C)CCOP(C)(=O)OCCC(C)(C)C
Mol. weight [g/mol]:	264.34
CAS:	116401-88-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.23		Crippen Method
logp	4.715		Crippen Method
mcvol	232.100	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=C116401888&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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