

Phosphonic acid, phenyl-, dibutyl ester

Inchi:	InChI=1S/C14H23O3P/c1-3-5-12-16-18(15,17-13-6-4-2)14-10-8-7-9-11-14/h7-11H,3-6,12
InchiKey:	YBBHHAFAFADNTQHQ-UHFFFAOYSA-N
Formula:	C14H23O3P
SMILES:	CCCCOP(=O)(OCCCC)c1ccccc1
Mol. weight [g/mol]:	270.30
CAS:	1024-34-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.62		Crippen Method
logp	4.138		Crippen Method
mcvol	222.430	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1024346&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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