

Phosphonous acid, phenyl-, dibutyl ester

Other names:	Dibutyl phenylphosphonate
Inchi:	InChI=1S/C14H23O2P/c1-3-5-12-15-17(16-13-6-4-2)14-10-8-7-9-11-14/h7-11H,3-6,12-14
InchiKey:	YBAAIJIDIRQVLY-UHFFFAOYSA-N
Formula:	C14H23O2P
SMILES:	CCCCOP(OCCCC)c1ccccc1
Mol. weight [g/mol]:	254.31
CAS:	3030-90-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.18		Crippen Method
logp	4.257		Crippen Method
mcvol	216.560	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3030908&Units=SI

Legend

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

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