

diethyl 4-chlorobenzylphosphonate

Inchi:	InChI=1S/C11H16ClO3P/c1-3-14-16(13,15-4-2)9-10-5-7-11(12)8-6-10/h5-8H,3-4,9H2,1-2
InchiKey:	BVQPVBRJSFOEZ-UHFFFAOYSA-N
Formula:	C11H16ClO3P
SMILES:	CCOP(=O)(Cc1ccc(Cl)cc1)OCC
Mol. weight [g/mol]:	262.67
CAS:	39225-17-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.16		Crippen Method
logp	4.106		Crippen Method
mcvol	192.400	ml/mol	McGowan Method

Sources

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=C39225177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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