

(p-Chloro-Benzoyl)-phosphonic acid diethyl ester

Inchi:	InChI=1S/C11H14ClO4P/c1-3-15-17(14,16-4-2)11(13)9-5-7-10(12)8-6-9/h5-8H,3-4H2,1-2H3
InchiKey:	VDKATAVRWLSKCS-UHFFFAOYSA-N
Formula:	C11H14ClO4P
SMILES:	CCOP(=O)(OCC)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	276.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.02		Crippen Method
logp	3.746		Crippen Method
mcvol	193.970	ml/mol	McGowan Method
rinpol	1811.00		NIST Webbook
rinpol	1821.00		NIST Webbook
rinpol	1811.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R205231&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
rinpol:	Non-polar retention indices

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