(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,3-4H2,1-2

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