(o-Methyl-Benzoyl)-phosphonic acid diethyl ester

Inchi: InChI=1S/C12H17O4P/c1-4-15-17(14,16-5-2)12(13)11-9-7-6-8-10(11)3/h6-9H,4-5H2,1-3

InchiKey: OWGXWFLJRBMYGI-UHFFFAOYSA-N

Formula: C12H17O4P

SMILES: CCOP(=O)(OCC)C(=O)c1ccccc1C

Mol. weight [g/mol]: 256.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.81		Crippen Method
logp	3.401		Crippen Method
mcvol	195.820	ml/mol	McGowan Method
rinpol	1711.00		NIST Webbook
rinpol	1724.00		NIST Webbook
rinpol	1711.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R205211&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices