Diethyl 4-methylphenyl phosphate

Inchi: InChI=1S/C11H17O4P/c1-4-13-16(12,14-5-2)15-11-8-6-10(3)7-9-11/h6-9H,4-5H2,1-3H3
InchiKey: UBSNERLLCAIDQQ-UHFFFAOYSA-N
Formula: C11H17O4P
SMILES: CCOP(=O)(OCC)Oc1ccc(C)cc1
Mol. weight [g/mol]: 244.22
CAS: 4877-08-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	3.555		Crippen Method
mcvol	186.030	ml/mol	McGowan Method
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
ripol	2310.00		NIST Webbook
ripol	2310.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4877081&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices