Dimethyl 3-methylphenyl phosphate

Inchi: InChI=1S/C9H13O4P/c1-8-5-4-6-9(7-8)13-14(10,11-2)12-3/h4-7H,1-3H3
InchiKey: BQGIVCKQWCUOME-UHFFFAOYSA-N
Formula: C9H13O4P
SMILES: COP(=O)(OC)Oc1cccc(C)c1
Mol. weight [g/mol]: 216.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.92		Crippen Method
logp	2.775		Crippen Method
mcvol	157.850	ml/mol	McGowan Method
rinpol	1488.00		NIST Webbook
ripol	2219.00		NIST Webbook

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=R168999&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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