Diethyl Benzoylmethylphosphonate

Inchi: InChI=1S/C12H17O4P/c1-3-15-17(14,16-4-2)10-12(13)11-8-6-5-7-9-11/h5-9H,3-4,10H2,
InchiKey: HPEVTTNSIPGLEL-UHFFFAOYSA-N
Formula: C12H17O4P
SMILES: CCOP(=O)(CC(=O)c1ccccc1)OCC
Mol. weight [g/mol]: 256.23
CAS: 3453-00-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.25		Crippen Method
logp	3.135		Crippen Method
mcvol	195.820	ml/mol	McGowan Method

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=C3453007&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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