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

Inchi: InChI=1S/C10H13O4P/c1-8-6-4-5-7-9(8)10(11)15(12,13-2)14-3/h4-7H,1-3H3
InchiKey: LFBRLNUGUVEMOG-UHFFFAOYSA-N
Formula: C10H13O4P
SMILES: COP(=O)(OC)C(=O)c1ccccc1C
Mol. weight [g/mol]: 228.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.97		Crippen Method
logp	2.621		Crippen Method
mcvol	167.640	ml/mol	McGowan Method
rinpol	1626.00		NIST Webbook
rinpol	1637.00		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=R205226&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

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