(p-Methoxy-Benzoyl)-phosphonic acid dimethyl ester

Inchi: InChI=1S/C10H13O5P/c1-13-9-6-4-8(5-7-9)10(11)16(12,14-2)15-3/h4-7H,1-3H3
InchiKey: TYYKVIUTXZKDQU-UHFFFAOYSA-N
Formula: C10H13O5P
SMILES: COc1ccc(C(=O)P(=O)(OC)OC)cc1
Mol. weight [g/mol]: 244.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	2.321		Crippen Method
mcvol	173.510	ml/mol	McGowan Method
rinpol	1859.00		NIST Webbook
rinpol	1871.00		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=R205266&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.