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

Inchi: InChI=1S/C12H17O5P/c1-4-16-18(14,17-5-2)12(13)10-6-8-11(15-3)9-7-10/h6-9H,4-5H2,

InchiKey: SDVRDVLYLCQGPF-UHFFFAOYSA-N

Formula: C12H17O5P

SMILES: CCOP(=O)(OCC)C(=O)c1ccc(OC)cc1

Mol. weight [g/mol]: 272.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.45		Crippen Method
logp	3.102		Crippen Method
mcvol	201.690	ml/mol	McGowan Method
rinpol	1952.00		NIST Webbook
rinpol	1964.00		NIST Webbook
rinpol	1952.00		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=R205251&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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