

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/ci9903071
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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