

Diethyl 2-methylbenzylphosphonate

Other names:	Diethyl O-methylbenzylphosphonate Phosphonic acid, [(2-methylphenyl)methyl]-, diethyl ester
Inchi:	InChI=1S/C12H19O3P/c1-4-14-16(13,15-5-2)10-12-9-7-6-8-11(12)3/h6-9H,4-5,10H2,1-3
InchiKey:	SAVIMLRKAZZCZ-UHFFFAOYSA-N
Formula:	C12H19O3P
SMILES:	CCOP(=O)(Cc1ccccc1C)OCC
Mol. weight [g/mol]:	242.25
CAS:	62778-16-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.95		Crippen Method
logp	3.761		Crippen Method
mcvol	194.250	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62778169&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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