

Phosphoramidic acid, (2,4-dimethylphenyl)-,diethyl ester

Inchi:	InChI=1S/C12H20NO3P/c1-5-15-17(14,16-6-2)13-12-8-7-10(3)9-11(12)4/h7-9H,5-6H2,1-
InchiKey:	YSPBUSSFSXCIMR-UHFFFAOYSA-N
Formula:	C12H20NO3P
SMILES:	CCOP(=O)(Nc1ccc(C)cc1C)OCC
Mol. weight [g/mol]:	257.27
CAS:	22767-82-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.13		Crippen Method
logp	3.896		Crippen Method
mcvol	204.230	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=C22767824&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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