

Phosphorous acid, methyl diphenyl ester

Inchi:	InChI=1S/C13H13O3P/c1-14-17(15-12-8-4-2-5-9-12)16-13-10-6-3-7-11-13/h2-11H,1H3
InchiKey:	NYCZNDFWFCCTPA-UHFFFAOYSA-N
Formula:	C13H13O3P
SMILES:	COP(Oc1ccccc1)Oc1ccccc1
Mol. weight [g/mol]:	248.21
CAS:	3577-87-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.85		Crippen Method
logp	4.018		Crippen Method
mcvol	184.580	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=C3577875&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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