

Phosphonous acid, phenyl-, diphenyl ester

Inchi:	InChI=1S/C18H15O2P/c1-4-10-16(11-5-1)19-21(18-14-8-3-9-15-18)20-17-12-6-2-7-13-1
InchiKey:	QXKPLZDCTKREIA-UHFFFAOYSA-N
Formula:	C18H15O2P
SMILES:	c1ccc(OP(Oc2ccccc2)c2ccccc2)cc1
Mol. weight [g/mol]:	294.28
CAS:	13410-61-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.36		Crippen Method
logp	4.782		Crippen Method
mcvol	225.400	ml/mol	McGowan Method

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=C13410612&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

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