

Phenyl phosphonic acid diphenyl ester

Other names:	diphenyl phenylphosphonate
Inchi:	InChI=1S/C18H15O3P/c19-22(18-14-8-3-9-15-18,20-16-10-4-1-5-11-16)21-17-12-6-2-7-
InchiKey:	CDOMXXVCZQOQMT-UHFFFAOYSA-N
Formula:	C18H15O3P
SMILES:	O=P(Oc1ccccc1)(Oc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	310.28
CAS:	3049-24-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.80		Crippen Method
logp	4.663		Crippen Method
mcvol	231.270	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=C3049249&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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