3-Methyl-1-phenyl-2-phospholene-1-oxide

Other names:	1H-Phosphole, 2,3-dihydro-4-methyl-1-phenyl-, 1-oxide
	2-Phospholene, 3-methyl-1-phenyl-, 1-oxide
	2,3-Dihydro-4-methyl-1-phenyl-1H-phosphole, 1-oxide
Inchi:	InChI=1S/C11H13OP/c1-10-7-8-13(12,9-10)11-5-3-2-4-6-11/h2-6,9H,7-8H2,1H3
InchiKey:	YMKWWHFRGALXLE-UHFFFAOYSA-N
Formula:	C11H13OP
SMILES:	CC1=CP(=O)(c2ccccc2)CC1
Mol. weight [g/mol]:	192.19
CAS:	707-61-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.45		Crippen Method
logp	2.982		Crippen Method
mcvol	153.260	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=C707619&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