1,3,2-Dioxaphosphorinane, 5,5-dimethyl-2-phenoxy-, 2-oxide

Other names: Phosphoric acid, cyclic 2,2-dimethyltrimethylene phenyl ester
Cyclic 2,2-dimethyltrimethylene phenyl phosphate
Phosphoric acid, phenyl (cyclic 2,2-dimethyltrimethylene) ester
1,3-Propanediol, 2,2-dimethyl-, cyclic phenyl phosphate
5,5-dimethyl-2-phenoxy-1,3,2-dioxaphosphorinane 2-oxide

Inchi: InChI=1S/C11H15O4P/c1-11(2)8-13-16(12,14-9-11)15-10-6-4-3-5-7-10/h3-7H,8-9H2,1-2

InchiKey: VSKVZTVOVPEFOH-UHFFFAOYSA-N

Formula: C11H15O4P

SMILES: CC1(C)COP(=O)(Oc2ccccc2)OC1

Mol. weight [g/mol]: 242.21

CAS: 884-89-9

Physical Properties

Property code	Value	Unit	Source
ie	9.00	eV	NIST Webbook
log10ws	-4.36		Crippen Method
logp	3.247		Crippen Method
mcvol	175.170	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=C884899&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume