Phosphorous acid, cyclic o-phenylene-, isobutyl ester

Inchi: InChI=1S/C10H13O3P/c1-8(2)7-11-14-12-9-5-3-4-6-10(9)13-14/h3-6,8H,7H2,1-2H3
InchiKey: HZAUOUTUWDZSGV-UHFFFAOYSA-N
Formula: C10H13O3P
SMILES: CC(C)COP1Oc2ccccc2O1
Mol. weight [g/mol]: 212.18
CAS: 4591-39-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.11		Crippen Method
logp	3.357		Crippen Method
mcvol	155.210	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=C4591393&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