Diallyl hydrogen phosphite

Inchi: InChI=1S/C6H11O3P/c1-3-5-8-10(7)9-6-4-2/h3-4,10H,1-2,5-6H2
InchiKey: XHJSDYZZKCDLFI-UHFFFAOYSA-N
Formula: C6H11O3P
SMILES: C=CCO[PH](=O)OCC=C
Mol. weight [g/mol]: 162.12
CAS: 23679-20-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Crippen Method
logp	1.781		Crippen Method
mcvol	124.870	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C23679201&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume