O-Ethyl-O-(1,1-difluoro-2-chloroethyl)-N-allyl-phos

Inchi: InChI=1S/C7H13ClF2NO2PS/c1-3-5-11-14(15,12-4-2)13-7(9,10)6-8/h3H,1,4-6H2,2H3,(H
InchiKey: PULAQOVPUWYGPP-UHFFFAOYSA-N
Formula: C7H13ClF2NO2PS
SMILES: C=CCNP(=S)(OCC)OC(F)(F)CCl
Mol. weight [g/mol]: 279.67

Physical Properties

Property code	Value	Unit	Source
log10ws	0.81		Crippen Method
logp	2.871		Crippen Method
mcvol	179.500	ml/mol	McGowan Method
rinpol	1419.00		NIST Webbook

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=R543969&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices