O-Ethyl-O-(1,1-difluoro-2-chloroethyl)-N-butyl-pho

Inchi: InChI=1S/C8H17ClF2NO2PS/c1-3-5-6-12-15(16,13-4-2)14-8(10,11)7-9/h3-7H2,1-2H3,(H
InchiKey: GFDVTWACOWHQRZ-UHFFFAOYSA-N
Formula: C8H17ClF2NO2PS
SMILES: CCCCNP(=S)(OCC)OC(F)(F)CCl
Mol. weight [g/mol]: 295.71

Physical Properties

Property code	Value	Unit	Source
log10ws	0.25		Crippen Method
logp	3.485		Crippen Method
mcvol	197.890	ml/mol	McGowan Method
rinpol	1530.00		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=R543974&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