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

Inchi: InChI=1S/C6H13ClF2NO2PS/c1-3-10-13(14,11-4-2)12-6(8,9)5-7/h3-5H2,1-2H3,(H,10,14
InchiKey: PXHGHKLCVUBPPM-UHFFFAOYSA-N
Formula: C6H13ClF2NO2PS
SMILES: CCNP(=S)(OCC)OC(F)(F)CCl
Mol. weight [g/mol]: 267.66

Physical Properties

Property code	Value	Unit	Source
log10ws	1.09		Crippen Method
logp	2.705		Crippen Method
mcvol	169.710	ml/mol	McGowan Method
rinpol	1353.00		NIST Webbook
rinpol	1353.00		NIST Webbook

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=R543989&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
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.