O-Ethyl-O-(1,1-difluoro-2-chloroethyl)-N-(1-methyl

Inchi: InChI=1S/C9H19ClF2NO2PS/c1-4-6-8(3)13-16(17,14-5-2)15-9(11,12)7-10/h8H,4-7H2,1-

InchiKey: BJUVCDYBBSBAAV-UHFFFAOYSA-N

Formula: C9H19ClF2NO2PS

SMILES: CCCC(C)NP(=S)(OCC)OC(F)(F)CCl

Mol. weight [g/mol]: 309.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.28		Crippen Method
logp	3.874		Crippen Method
mcvol	211.980	ml/mol	McGowan Method
rinpol	1462.00		NIST Webbook
rinpol	1462.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R543954&Units=SI

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

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.