O-Methyl-O-(1,1-difluoro-2-chloroethyl)-N-(1-ethyl

Inchi: InChI=1S/C8H17ClF2NO2PS/c1-4-7(5-2)12-15(16,13-3)14-8(10,11)6-9/h7H,4-6H2,1-3H3
InchiKey: AEFUQFDCGMMPQM-UHFFFAOYSA-N
Formula: C8H17ClF2NO2PS
SMILES: CCC(CC)NP(=S)(OC)OC(F)(F)CCl
Mol. weight [g/mol]: 295.71

Physical Properties

Property code	Value	Unit	Source
log10ws	0.14		Crippen Method
logp	3.484		Crippen Method
mcvol	197.890	ml/mol	McGowan Method
rinpol	1497.00		NIST Webbook
rinpol	1497.00		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=R544140&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.