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

Inchi: InChI=1S/C8H15ClF2NO2PS/c1-13-15(16,14-8(10,11)6-9)12-7-4-2-3-5-7/h7H,2-6H2,1H3
InchiKey: BGELSJDJUNLXNU-UHFFFAOYSA-N
Formula: C8H15ClF2NO2PS
SMILES: COP(=S)(NC1CCCC1)OC(F)(F)CCl
Mol. weight [g/mol]: 293.70

Physical Properties

Property code	Value	Unit	Source
log10ws	0.24		Crippen Method
logp	3.238		Crippen Method
mcvol	187.030	ml/mol	McGowan Method
rinpol	1613.00		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=R544195&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