O-(2-Chloro-1,1-difluoroethyl)-N,N-diethylamidoet

Inchi: InChI=1S/C8H17ClF2NOPS/c1-4-12(5-2)14(15,6-3)13-8(10,11)7-9/h4-7H2,1-3H3
InchiKey: SGWGGNJKCAYXGO-UHFFFAOYSA-N
Formula: C8H17ClF2NOPS
SMILES: CCN(CC)P(=S)(CC)OC(F)(F)CCl
Mol. weight [g/mol]: 279.71

Physical Properties

Property code	Value	Unit	Source
log10ws	0.95		Crippen Method
logp	3.506		Crippen Method
mcvol	192.020	ml/mol	McGowan Method
rinpol	1469.00		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=R544511&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