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

Inchi: InChI=1S/C7H15ClF2NO2PS/c1-3-5-11-14(12,15-4-2)13-7(9,10)6-8/h3-6H2,1-2H3,(H,11
InchiKey: VZXIORFQKSTSKD-UHFFFAOYSA-N
Formula: C7H15ClF2NO2PS
SMILES: CCCNP(=O)(OC(F)(F)CCl)SCC
Mol. weight [g/mol]: 281.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Crippen Method
logp	3.695		Crippen Method
mcvol	183.800	ml/mol	McGowan Method
rinpol	1397.00		NIST Webbook
rinpol	1461.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R544417&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.