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

Inchi: InChI=1S/C6H13ClF2NOPS/c1-3-4-10-12(2,13)11-6(8,9)5-7/h3-5H2,1-2H3,(H,10,13)
InchiKey: HQMHMJIJRPHHDX-UHFFFAOYSA-N
Formula: C6H13ClF2NOPS
SMILES: CCCNP(C)(=S)OC(F)(F)CCl
Mol. weight [g/mol]: 251.66

Physical Properties

Property code	Value	Unit	Source
log10ws	1.16		Crippen Method
logp	2.773		Crippen Method
mcvol	163.840	ml/mol	McGowan Method
rinpol	1384.00		NIST Webbook
rinpol	1384.00		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=R544531&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

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