O-Ethyl-O-(2-chloro-1,1-difluoroethyl)methanethio

Inchi: InChI=1S/C5H10ClF2O2PS/c1-3-9-11(2,12)10-5(7,8)4-6/h3-4H2,1-2H3
InchiKey: DGNSJLHZONEDKH-UHFFFAOYSA-N
Formula: C5H10ClF2O2PS
SMILES: CCOP(C)(=S)OC(F)(F)CCl
Mol. weight [g/mol]: 238.62

Physical Properties

Property code	Value	Unit	Source
log10ws	1.68		Crippen Method
logp	2.810		Crippen Method
mcvol	145.640	ml/mol	McGowan Method
rinpol	1141.00		NIST Webbook
rinpol	1141.00		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=R544566&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.