O,O-Diethyl-S-(1,1-difluoro-2-chloroethyl)-dithiopl

Inchi: InChI=1S/C6H12ClF2O2PS2/c1-3-10-12(13,11-4-2)14-6(8,9)5-7/h3-5H2,1-2H3
InchiKey: NVWVCHLLCXCQSA-UHFFFAOYSA-N
Formula: C6H12ClF2O2PS2
SMILES: CCOP(=S)(OCC)SC(F)(F)CCl
Mol. weight [g/mol]: 284.71

Physical Properties

Property code	Value	Unit	Source
log10ws	0.39		Crippen Method
logp	3.849		Crippen Method
mcvol	176.080	ml/mol	McGowan Method
rinpol	1360.00		NIST Webbook
rinpol	1360.00		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=R544368&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.