O-Ethyl-O-isopropyl-S-(1,1-difluoroethyl)-dithioph

Inchi: InChI=1S/C7H15F2O2PS2/c1-5-10-12(13,11-6(2)3)14-7(4,8)9/h6H,5H2,1-4H3
InchiKey: OEQSWVFQJYTIDL-UHFFFAOYSA-N
Formula: C7H15F2O2PS2
SMILES: CCOP(=S)(OC(C)C)SC(C)(F)F
Mol. weight [g/mol]: 264.29

Physical Properties

Property code	Value	Unit	Source
log10ws	0.01		Crippen Method
logp	4.018		Crippen Method
mcvol	177.930	ml/mol	McGowan Method
rinpol	1282.00		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=R544333&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