O-Ethyl-O-isobutyl-S-(1,1-difluoroethyl)-dithiopho

Inchi: InChI=1S/C8H17F2O2PS2/c1-5-11-13(14,12-6-7(2)3)15-8(4,9)10/h7H,5-6H2,1-4H3
InchiKey: HBGGOWHQEDSGIH-UHFFFAOYSA-N
Formula: C8H17F2O2PS2
SMILES: CCOP(=S)(OCC(C)C)SC(C)(F)F
Mol. weight [g/mol]: 278.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.05		Crippen Method
logp	4.266		Crippen Method
mcvol	192.020	ml/mol	McGowan Method
rinpol	1375.00		NIST Webbook
rinpol	1375.00		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=R544328&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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