O,O-Diisobutyl-S-(1,1-difluoroethyl)-dithiophosph

Inchi: InChI=1S/C10H21F2O2PS2/c1-8(2)6-13-15(16,14-7-9(3)4)17-10(5,11)12/h8-9H,6-7H2,1
InchiKey: QYXOZRSLDDSIKZ-UHFFFAOYSA-N
Formula: C10H21F2O2PS2
SMILES: CC(C)COP(=S)(OCC(C)C)SC(C)(F)F
Mol. weight [g/mol]: 306.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.65		Crippen Method
logp	4.902		Crippen Method
mcvol	220.200	ml/mol	McGowan Method
rinpol	1499.00		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=R544388&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