O-isobutyl-S-(1,1-difluoroethyl)-dithioethylphosph

Inchi: InChI=1S/C8H17F2OPS2/c1-5-12(13,11-6-7(2)3)14-8(4,9)10/h7H,5-6H2,1-4H3
InchiKey: RRJGYPZQZDQDQE-UHFFFAOYSA-N
Formula: C8H17F2OPS2
SMILES: CCP(=S)(OCC(C)C)SC(C)(F)F
Mol. weight [g/mol]: 262.32

Physical Properties

Property code	Value	Unit	Source
log10ws	0.03		Crippen Method
logp	4.334		Crippen Method
mcvol	186.150	ml/mol	McGowan Method
rinpol	1384.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R544353&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices