O-Methyl-O-(1,1-difluoro-2-chloroethyl)-N-isobuty

Inchi: InChI=1S/C7H15ClF2NO2PS/c1-6(2)4-11-14(15,12-3)13-7(9,10)5-8/h6H,4-5H2,1-3H3,(H
InchiKey: VHUTYZWAWNGIAN-UHFFFAOYSA-N
Formula: C7H15ClF2NO2PS
SMILES: COP(=S)(NCC(C)C)OC(F)(F)CCl
Mol. weight [g/mol]: 281.69

Physical Properties

Property code	Value	Unit	Source
log10ws	0.91		Crippen Method
logp	2.951		Crippen Method
mcvol	183.800	ml/mol	McGowan Method
rinpol	1432.00		NIST Webbook
rinpol	1432.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R544224&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.