O-Methyl-O-(1,1-difluoro-2-bromoethyl)-N-isoprop

Inchi: InChI=1S/C6H13BrF2NO2PS/c1-5(2)10-13(14,11-3)12-6(8,9)4-7/h5H,4H2,1-3H3,(H,10,1
InchiKey: VLCMGTLEMVBHAG-UHFFFAOYSA-N
Formula: C6H13BrF2NO2PS
SMILES: COP(=S)(NC(C)C)OC(F)(F)CBr
Mol. weight [g/mol]: 312.11

Physical Properties

Property code	Value	Unit	Source
log10ws	0.70		Crippen Method
logp	2.860		Crippen Method
mcvol	174.970	ml/mol	McGowan Method
rinpol	1398.00		NIST Webbook
rinpol	1398.00		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=R544091&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.