O-(2-Bromo-1,1-difluoroethyl)-N-isopropylamidoe

Inchi: InChI=1S/C7H15BrF2NOPS/c1-4-13(14,11-6(2)3)12-7(9,10)5-8/h6H,4-5H2,1-3H3,(H,11,
InchiKey: HJGXLETWGWFFTQ-UHFFFAOYSA-N
Formula: C7H15BrF2NOPS
SMILES: CCP(=S)(NC(C)C)OC(F)(F)CBr
Mol. weight [g/mol]: 310.14

Physical Properties

Property code	Value	Unit	Source
log10ws	0.35		Crippen Method
logp	3.318		Crippen Method
mcvol	183.190	ml/mol	McGowan Method
rinpol	1485.00		NIST Webbook
rinpol	1485.00		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=R544442&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.