O-(2-Bromo-1,1-difluoroethyl)-N-(1-methylpropyl)a

Inchi: InChI=1S/C8H17BrF2NOPS/c1-4-7(3)12-14(15,5-2)13-8(10,11)6-9/h7H,4-6H2,1-3H3,(H,
InchiKey: IXKJSYDRUCTKEI-UHFFFAOYSA-N
Formula: C8H17BrF2NOPS
SMILES: CCC(C)NP(=S)(CC)OC(F)(F)CBr
Mol. weight [g/mol]: 324.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.06		Crippen Method
logp	3.708		Crippen Method
mcvol	197.280	ml/mol	McGowan Method
rinpol	1578.00		NIST Webbook
rinpol	1578.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R544437&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

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