O-Ethyl-O-(2-bromo-1,1-difluoroethyl)ethanethion

Inchi: InChI=1S/C4H7BrClF2O2PS/c1-2-9-11(6,12)10-4(7,8)3-5/h2-3H2,1H3
InchiKey: ADHCOHPXVVZZNJ-UHFFFAOYSA-N
Formula: C4H7BrClF2O2PS
SMILES: CCOP(=S)(Cl)OC(F)(F)CBr
Mol. weight [g/mol]: 303.49

Physical Properties

Property code	Value	Unit	Source
log10ws	0.68		Crippen Method
logp	3.491		Crippen Method
mcvol	149.050	ml/mol	McGowan Method
rinpol	1301.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R544546&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