O-(2-Bromo-1,1-difluoroethyl)ethanechlorothiono

Inchi: InChI=1S/C4H7BrClF2OPS/c1-2-10(6,11)9-4(7,8)3-5/h2-3H2,1H3
InchiKey: ZHMVIVOJUHEZNL-UHFFFAOYSA-N
Formula: C4H7BrClF2OPS
SMILES: CCP(=S)(Cl)OC(F)(F)CBr
Mol. weight [g/mol]: 287.49

Physical Properties

Property code	Value	Unit	Source
log10ws	0.76		Crippen Method
logp	3.559		Crippen Method
mcvol	143.180	ml/mol	McGowan Method
rinpol	1242.00		NIST Webbook
rinpol	1242.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R544422&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

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