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

Inchi: InChI=1S/C2H2BrCl2F2OPS/c3-1-2(6,7)8-9(4,5)10/h1H2
InchiKey: LZNNSOAIPYJQQB-UHFFFAOYSA-N
Formula: C2H2BrCl2F2OPS
SMILES: FC(F)(CBr)OP(=S)(Cl)Cl
Mol. weight [g/mol]: 293.88

Physical Properties

Property code	Value	Unit	Source
log10ws	0.45		Crippen Method
logp	3.693		Crippen Method
mcvol	127.240	ml/mol	McGowan Method
rinpol	1119.00		NIST Webbook
rinpol	1119.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R543909&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

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