O-Methyl-O-(1,1-difluoro-2-bromoethyl)-N-metyl-p

Inchi: InChI=1S/C4H9BrF2NO2PS/c1-8-11(12,9-2)10-4(6,7)3-5/h3H2,1-2H3,(H,8,12)
InchiKey: NODCHCMKYCUBPJ-UHFFFAOYSA-N
Formula: C4H9BrF2NO2PS
SMILES: CNP(=S)(OC)OC(F)(F)CBr
Mol. weight [g/mol]: 284.06

Physical Properties

Property code	Value	Unit	Source
log10ws	1.64		Crippen Method
logp	2.081		Crippen Method
mcvol	146.790	ml/mol	McGowan Method
rinpol	1339.00		NIST Webbook

Sources

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=R544100&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices