O-Ethyl-O-(1,1-difluoro-2-bromoethyl)-N-metyl-ph

Inchi: InChI=1S/C5H11BrF2NO2PS/c1-3-10-12(13,9-2)11-5(7,8)4-6/h3-4H2,1-2H3,(H,9,13)
InchiKey: BFRDNBWHSGEKNI-UHFFFAOYSA-N
Formula: C5H11BrF2NO2PS
SMILES: CCOP(=S)(NC)OC(F)(F)CBr
Mol. weight [g/mol]: 298.09

Physical Properties

Property code	Value	Unit	Source
log10ws	1.23		Crippen Method
logp	2.471		Crippen Method
mcvol	160.880	ml/mol	McGowan Method
rinpol	1388.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R543934&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