O-Methyl-O-(1,1-difluoro-2-bromoethyl)-N-allyl-ph

Inchi: InChI=1S/C6H11BrF2NO2PS/c1-3-4-10-13(14,11-2)12-6(8,9)5-7/h3H,1,4-5H2,2H3,(H,10
InchiKey: YWKJAAKQPQQFIA-UHFFFAOYSA-N
Formula: C6H11BrF2NO2PS
SMILES: C=CCNP(=S)(OC)OC(F)(F)CBr
Mol. weight [g/mol]: 310.10

Physical Properties

Property code	Value	Unit	Source
log10ws	0.95		Crippen Method
logp	2.637		Crippen Method
mcvol	170.670	ml/mol	McGowan Method
rinpol	1447.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R544086&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