O-Ethyl-O-(1,1-difluoro-2-bromoethyl)-N-(1-methyl

Inchi: InChI=1S/C8H17BrF2NO2PS/c1-4-7(3)12-15(16,13-5-2)14-8(10,11)6-9/h7H,4-6H2,1-3H3

InchiKey: SQHFWUNHKIIIGM-UHFFFAOYSA-N

Formula: C8H17BrF2NO2PS

SMILES: CCOP(=S)(NC(C)CC)OC(F)(F)CBr

Mol. weight [g/mol]: 340.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.14		Crippen Method
logp	3.640		Crippen Method
mcvol	203.150	ml/mol	McGowan Method
rinpol	1545.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1545.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R543929&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices