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

Inchi: InChI=1S/C7H15BrF2NO2PS/c1-3-5-11-14(15,12-4-2)13-7(9,10)6-8/h3-6H2,1-2H3,(H,11
InchiKey: DKAOYPOYYZCGPT-UHFFFAOYSA-N
Formula: C7H15BrF2NO2PS
SMILES: CCCNP(=S)(OCC)OC(F)(F)CBr
Mol. weight [g/mol]: 326.14

Physical Properties

Property code	Value	Unit	Source
log10ws	0.39		Crippen Method
logp	3.251		Crippen Method
mcvol	189.060	ml/mol	McGowan Method
rinpol	1518.00		NIST Webbook
rinpol	1558.00		NIST Webbook
rinpol	1518.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R543870&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