

O-Ethyl-O-(1,1-difluoro-2-chloroethyl)-N-methyl-p

Inchi: InChI=1S/C5H11ClF2NO2PS/c1-3-10-12(13,9-2)11-5(7,8)4-6/h3-4H2,1-2H3,(H,9,13)
InchiKey: BUXZBEJRYIAOGB-UHFFFAOYSA-N
Formula: C5H11ClF2NO2PS
SMILES: CCOP(=S)(NC)OC(F)(F)CCI
Mol. weight [g/mol]: 253.63

Physical Properties

Property code	Value	Unit	Source
log10ws	1.50		Crippen Method
logp	2.315		Crippen Method
mcvol	155.620	ml/mol	McGowan Method
rinpol	1308.00		NIST Webbook
rinpol	1308.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R544011&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

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