

O-Methyl-O-(1,1-difluoro-2-chloroethyl)-N-propyl-

Inchi:	InChI=1S/C6H13ClF2NO2PS/c1-3-4-10-13(14,11-2)12-6(8,9)5-7/h3-5H2,1-2H3,(H,10,14)
InchiKey:	ZRETZITYXUCEAL-UHFFFAOYSA-N
Formula:	C6H13ClF2NO2PS
SMILES:	CCCNP(=S)(OC)OC(F)(F)CCl
Mol. weight [g/mol]:	267.66

Physical Properties

Property code	Value	Unit	Source
log10ws	1.09		Crippen Method
logp	2.705		Crippen Method
mcvol	169.710	ml/mol	McGowan Method
rinpol	1387.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R544284&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

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