

O-Methyl-O-(1,1-difluoro-2-chloroethyl)-N-pentyl-p

Inchi:	InChI=1S/C8H17CIF2NO2PS/c1-3-4-5-6-12-15(16,13-2)14-8(10,11)7-9/h3-7H2,1-2H3,(H
InchiKey:	IBIMROVJNXHMJB-UHFFFAOYSA-N
Formula:	C8H17CIF2NO2PS
SMILES:	CCCCCNP(=S)(OC)OC(F)(F)CCI
Mol. weight [g/mol]:	295.71

Physical Properties

Property code	Value	Unit	Source
log10ws	0.25		Crippen Method
logp	3.485		Crippen Method
mcvol	197.890	ml/mol	McGowan Method
rinpola	1581.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R544279&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
rinpola:	Non-polar retention indices

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