

O-Methyl-O-(1,1-difluoro-2-bromoethyl)-N-allyl-ph

Inchi:	InChI=1S/C6H11BrF2NO2PS/c1-3-4-10-13(14,11-2)12-6(8,9)5-7/h3H,1,4-5H2,2H3,(H,10)
InchiKey:	YWKJAAKQPQQFIA-UHFFFAOYSA-N
Formula:	C6H11BrF2NO2PS
SMILES:	C=CCNP(=S)(OC)OC(F)(F)CBr
Mol. weight [g/mol]:	310.10

Physical Properties

Property code	Value	Unit	Source
log10ws	0.95		Crippen Method
logp	2.637		Crippen Method
mcvol	170.670	ml/mol	McGowan Method
rinpola	1447.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R544086&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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