O-(2-Bromo-1,1-difluoroethyl)-N,N-diethylamidoet

Inchi:	InChI=1S/C8H17BrF2NOPS/c1-4-12(5-2)14(15,6-3)13-8(10,11)7-9/h4-7H2,1-3H3
InchiKey:	DAPNLGUFTSZMSO-UHFFFAOYSA-N
Formula:	C8H17BrF2NOPS
SMILES:	CCN(CC)P(=S)(CC)OC(F)(F)CBr
Mol. weight [g/mol]:	324.17

Physical Properties

Property code	Value	Unit	Source
log10ws	0.67		Crippen Method
logp	3.662		Crippen Method
mcvol	197.280	ml/mol	McGowan Method
rinpol	1548.00		NIST Webbook
rinpol	1548.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R544457&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

Latest version available from:
https://www.chemeo.com/cid/33-623-3/O-2-Bromo-1-1-difluoroethyl-N-N-diethylamidoethanethionophosphonate.pdf
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