

O-Ethyl-O-(2-bromo-1,1-difluoroethyl)ethanethion

Inchi:	InChI=1S/C4H7BrClF2O2PS/c1-2-9-11(6,12)10-4(7,8)3-5/h2-3H2,1H3
InchiKey:	ADHCOHPXVVZZNJ-UHFFFAOYSA-N
Formula:	C4H7BrClF2O2PS
SMILES:	CCOP(=S)(Cl)OC(F)(F)CBr
Mol. weight [g/mol]:	303.49

Physical Properties

Property code	Value	Unit	Source
log10ws	0.68		Crippen Method
logp	3.491		Crippen Method
mcvol	149.050	ml/mol	McGowan Method
rinpola	1301.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R544546&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpola:	Non-polar retention indices

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