

O-Ethyl-O-(2-chloro-1,1-difluoroethyl)ethanethiop

Inchi: InChI=1S/C6H12ClF2O2PS/c1-3-10-12(13,4-2)11-6(8,9)5-7/h3-5H2,1-2H3
InchiKey: KWOFQUVNFMBBI-UHFFFAOYSA-N
Formula: C6H12ClF2O2PS
SMILES: CCOP(=S)(CC)OC(F)(F)CCI
Mol. weight [g/mol]: 252.65

Physical Properties

Property code	Value	Unit	Source
log10ws	1.27		Crippen Method
logp	3.200		Crippen Method
mcvol	159.730	ml/mol	McGowan Method
rinpol	1223.00		NIST Webbook
rinpol	1223.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R544551&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpol: Non-polar retention indices

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<https://www.cheméo.com/cid/67-533-6/O-Ethyl-O-2-chloro-1-1-difluoroethyl-ethanethiophosphonate.pdf>

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