

# O-(2-Chloro-1,1-difluoroethyl)-N-isopropylamidomethanethionophosphonate

<b>Inchi:</b>	InChI=1S/C6H13CIF2NOPS/c1-5(2)10-12(3,13)11-6(8,9)4-7/h5H,4H2,1-3H3,(H,10,13)
<b>InchiKey:</b>	VUJWVLSUZPYMHE-UHFFFAOYSA-N
<b>Formula:</b>	C6H13CIF2NOPS
<b>SMILES:</b>	CC(C)NP(C)(=S)OC(F)(F)CCI
<b>Mol. weight [g/mol]:</b>	251.66

## Physical Properties

Property code	Value	Unit	Source
log10ws	1.05		Crippen Method
logp	2.772		Crippen Method
mcvol	163.840	ml/mol	McGowan Method
rinpole	1325.00		NIST Webbook
rinpole	1325.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R544506&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R544506&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpole:</b>	Non-polar retention indices

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