

O-(2-Chloro-1,1-difluoroethyl)-N-(1-methylpropyl)amidoethanethionophosphonic acid

Inchi: InChI=1S/C8H17CIF2NOPS/c1-4-7(3)12-14(15,5-2)13-8(10,11)6-9/h7H,4-6H2,1-3H3,(H,)
InchiKey: RPEHXZPTBLMALG-UHFFFAOYSA-N
Formula: C8H17CIF2NOPS
SMILES: CCC(C)NP(=S)(CC)OC(F)(F)CCI
Mol. weight [g/mol]: 279.71

Physical Properties

Property code	Value	Unit	Source
log10ws	0.21		Crippen Method
logp	3.552		Crippen Method
mcvol	192.020	ml/mol	McGowan Method
rinsol	1496.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R544482&Units=SI>

Legend

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

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