O-(2-Chloro-1,1-difluoroethyl)methanechlorothion

Inchi: InChI=1S/C3H5Cl2F2OPS/c1-9(5,10)8-3(6,7)2-4/h2H2,1H3
InchiKey: BDHGZXAJVIXBMB-UHFFFAOYSA-N
Formula: C3H5Cl2F2OPS
SMILES: CP(=S)(Cl)OC(F)(F)CCl
Mol. weight [g/mol]: 229.01

Physical Properties

Property code	Value	Unit	Source
log10ws	1.46		Crippen Method
logp	3.013		Crippen Method
mcvol	123.830	ml/mol	McGowan Method
rinpol	1072.00		NIST Webbook
rinpol	1072.00		NIST Webbook

Sources

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=R544477&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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