

O-(1,1-Difluoro-2-chloroethyl)-phosphorothiodichloride

Inchi: InChI=1S/C2H2Cl3F2OPS/c3-1-2(6,7)8-9(4,5)10/h1H2
InchiKey: CEKVBWJYZVZRKR-UHFFFAOYSA-N
Formula: C2H2Cl3F2OPS
SMILES: FC(F)(CCI)OP(=S)(Cl)Cl
Mol. weight [g/mol]: 249.43

Physical Properties

Property code	Value	Unit	Source
log10ws	0.73		Crippen Method
logp	3.537		Crippen Method
mcvol	121.980	ml/mol	McGowan Method
rinpol	1037.00		NIST Webbook
rinpol	1037.00		NIST Webbook

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=R543890&Units=SI>

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/32-007-8/O-1-1-Difluoro-2-chloroethyl-phosphorothiodichloridate.pdf>

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