

O-Methyl-O-(1,1-difluoro-2-chloroethyl)-N,N-diethylphosphorothioamidate

Inchi: InChI=1S/C7H15ClF2NO2PS/c1-4-11(5-2)14(15,12-3)13-7(9,10)6-8/h4-6H2,1-3H3
InchiKey: JETGDLGBBFJEHV-UHFFFAOYSA-N
Formula: C7H15ClF2NO2PS
SMILES: CCN(CC)P(=S)(OC)OC(F)(F)CCI
Mol. weight [g/mol]: 281.69

Physical Properties

Property code	Value	Unit	Source
log10ws	1.29		Crippen Method
logp	3.047		Crippen Method
mcvol	183.800	ml/mol	McGowan Method
rmpol	1374.00		NIST Webbook
rmpol	1374.00		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=R544259&Units=SI>

Legend

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

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