O-(2-Chloro-1,1-difluoroethyl)-N,N-diethylamidom

Inchi: InChI=1S/C7H15ClF2NOPS/c1-4-11(5-2)13(3,14)12-7(9,10)6-8/h4-6H2,1-3H3
InchiKey: SEEHQBCMDLEFIV-UHFFFAOYSA-N
Formula: C7H15ClF2NOPS
SMILES: CCN(CC)P(C)(=S)OC(F)(F)CCl
Mol. weight [g/mol]: 265.69

Physical Properties

Property code	Value	Unit	Source
log10ws	1.36		Crippen Method
logp	3.116		Crippen Method
mcvol	177.930	ml/mol	McGowan Method
rinpol	1387.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R544526&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.chemeo.com/cid/32-218-4/O-2-Chloro-1-1-difluoroethyl-N-N-diethylamidomethanethionophosphonate.pd
Generated by Cheméo on 2024-04-20 11:21:18.408921715 +0000 UTC m=+15901327.329499032.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.