

O-Ethyl-O-(1,1-difluoro-2-chloroethyl)-N,N-diethyl-

Inchi:	InChI=1S/C8H17ClF2NO2PS/c1-4-12(5-2)15(16,13-6-3)14-8(10,11)7-9/h4-7H2,1-3H3
InchiKey:	PWSNPGPFBDKFCI-UHFFFAOYSA-N
Formula:	C8H17ClF2NO2PS
SMILES:	CCOP(=S)(OC(F)(F)CC)N(CC)CC
Mol. weight [g/mol]:	295.71

Physical Properties

Property code	Value	Unit	Source
log10ws	0.87		Crippen Method
logp	3.437		Crippen Method
mcvol	197.890	ml/mol	McGowan Method
rinpol	1416.00		NIST Webbook
rinpol	1416.00		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=R544026&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

Latest version available from:

<https://www.chemeo.com/cid/118-118-0/O-Ethyl-O-1-1-difluoro-2-chloroethyl-N-N-diethyl-phosphorothioamidate.pdf>

Generated by Cheméo on 2024-04-30 23:44:49.142199504 +0000 UTC m=+16809938.062776819.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.