O-Methyl-O-(1,1-difluoro-2-chloroethyl)-phosphor

Inchi: InChI=1S/C3H5Cl2F2O2PS/c1-8-10(5,11)9-3(6,7)2-4/h2H2,1H3
InchiKey: QTXYEXINXCBBHX-UHFFFAOYSA-N
Formula: C3H5Cl2F2O2PS
SMILES: COP(=S)(Cl)OC(F)(F)CCl
Mol. weight [g/mol]: 245.01

Physical Properties

Property code	Value	Unit	Source
log10ws	1.38		Crippen Method
logp	2.944		Crippen Method
mcvol	129.700	ml/mol	McGowan Method
rinpol	1104.00		NIST Webbook
rinpol	1104.00		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=R544299&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

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