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

Inchi: InChI=1S/C3H5BrClF2O2PS/c1-8-10(5,11)9-3(6,7)2-4/h2H2,1H3
InchiKey: QMECABHJLBKPLL-UHFFFAOYSA-N
Formula: C3H5BrClF2O2PS
SMILES: COP(=S)(Cl)OC(F)(F)CBr
Mol. weight [g/mol]: 289.46

Physical Properties

Property code	Value	Unit	Source
log10ws	1.10		Crippen Method
logp	3.100		Crippen Method
mcvol	134.960	ml/mol	McGowan Method
rinpol	1180.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R544120&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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