O-Ethyl-S-(1,1-difluoroethyl)-dithioethylphosphon

Inchi: InChI=1S/C6H13F2OPS2/c1-4-9-10(11,5-2)12-6(3,7)8/h4-5H2,1-3H3
InchiKey: DXFKGLKBLPPVDL-UHFFFAOYSA-N
Formula: C6H13F2OPS2
SMILES: CCOP(=S)(CC)SC(C)(F)F
Mol. weight [g/mol]: 234.27

Physical Properties

Property code	Value	Unit	Source
log10ws	0.62		Crippen Method
logp	3.698		Crippen Method
mcvol	157.970	ml/mol	McGowan Method
rinpol	1249.00		NIST Webbook
rinpol	1249.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R544348&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

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