

O,O-Dimethyl-S-(1,1-difluoroethyl)-dithiophosphate

Inchi: InChI=1S/C4H9F2O2PS2/c1-4(5,6)11-9(10,7-2)8-3/h1-3H3
InchiKey: QXMWWCXQKCPJDV-UHFFFAOYSA-N
Formula: C4H9F2O2PS2
SMILES: COP(=S)(OC)SC(C)(F)F
Mol. weight [g/mol]: 222.21

Physical Properties

Property code	Value	Unit	Source
log10ws	1.38		Crippen Method
logp	2.850		Crippen Method
mcvol	135.660	ml/mol	McGowan Method
rinpole	1133.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R544402&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/50-720-6/O-O-Dimethyl-S-1-1-difluoroethyl-dithiophosphate.pdf>

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