

O-(4-Chlorophenyl)-S-(1,1-difluoroethyl)-dithioeth

Inchi:	InChI=1S/C10H12ClF2OPS2/c1-3-15(16,17-10(2,12)13)14-9-6-4-8(11)5-7-9/h4-7H,3H2,1
InchiKey:	NJVIDQLYXHXZBZ-UHFFFAOYSA-N
Formula:	C10H12ClF2OPS2
SMILES:	CCP(=S)(Oc1ccc(Cl)cc1)SC(C)(F)F
Mol. weight [g/mol]:	316.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	5.394		Crippen Method
mcvol	202.810	ml/mol	McGowan Method
rinpol	1861.00		NIST Webbook
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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=R544308&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/30-274-4/O-4-Chlorophenyl-S-1-1-difluoroethyl-dithioethylphosphonate.pdf>

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