

O-isobutyl-S-(1,1-difluoroethyl)-dithioethylphosphonate

Inchi:	InChI=1S/C8H17F2OPS2/c1-5-12(13,11-6-7(2)3)14-8(4,9)10/h7H,5-6H2,1-4H3
InchiKey:	RRJGYPZQZDQDQE-UHFFFAOYSA-N
Formula:	C8H17F2OPS2
SMILES:	CCP(=S)(OCC(C)C)SC(C)(F)F
Mol. weight [g/mol]:	262.32

Physical Properties

Property code	Value	Unit	Source
log10ws	0.03		Crippen Method
logp	4.334		Crippen Method
mcvol	186.150	ml/mol	McGowan Method
rinpol	1384.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R544353&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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