O-Ethyl-O-isobutyl-S-(1,1-difluoro-3-ethylheptyl)-d

Inchi: InChI=1S/C15H31F2O2PS2/c1-6-9-10-14(7-2)11-15(16,17)22-20(21,18-8-3)19-12-13(4)5

InchiKey: OWSWVZBOYCVPHR-UHFFFAOYSA-N

Formula: C15H31F2O2PS2

SMILES: CCCCC(CC)CC(F)(F)SP(=S)(OCC)OCC(C)C

Mol. weight [g/mol]: 376.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	6.853		Crippen Method
mcvol	290.650	ml/mol	McGowan Method
rinpol	1846.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R544313&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

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