

O-Ethyl-O-(1,1-difluoro-2-bromoethyl)-N-(1-methyl)

Inchi: InChI=1S/C8H17BrF2NO2PS/c1-4-7(3)12-15(16,13-5-2)14-8(10,11)6-9/h7H,4-6H2,1-3H3
InchiKey: SQHFWUNHKIIIIGM-UHFFFAOYSA-N
Formula: C8H17BrF2NO2PS
SMILES: CCOP(=S)(NC(C)CC)OC(F)(F)CBr
Mol. weight [g/mol]: 340.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.14		Crippen Method
logp	3.640		Crippen Method
mcvol	203.150	ml/mol	McGowan Method
rinpol	1545.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1545.00		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=R543929&Units=SI>

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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<https://www.chemeo.com/cid/36-417-9/O-Ethyl-O-1-1-difluoro-2-bromoethyl-N-1-methylpropyl-phosphorothioamidate>

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