

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

Inchi:	InChI=1S/C5H11BrF2NO2PS/c1-3-10-12(13,9-2)11-5(7,8)4-6/h3-4H2,1-2H3,(H,9,13)
InchiKey:	BFRDNBWHSGEKNI-UHFFFAOYSA-N
Formula:	C5H11BrF2NO2PS
SMILES:	CCOP(=S)(NC)OC(F)(F)CBr
Mol. weight [g/mol]:	298.09

Physical Properties

Property code	Value	Unit	Source
log10ws	1.23		Crippen Method
logp	2.471		Crippen Method
mcvol	160.880	ml/mol	McGowan Method
rinpol	1388.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R543934&Units=SI
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

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/25-753-8/O-Ethyl-O-1-1-difluoro-2-bromoethyl-N-methyl-phosphorothioamidate.pdf>

Generated by Cheméo on 2024-05-01 02:38:06.838922027 +0000 UTC m=+16820335.759499343.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.