Urea, 1-(2-fluoroethyl)-1-nitroso-3-(1,2,3,4-tetrahydro-2,4

Inchi: InChI=1S/C7H8FN5O4/c8-1-2-13(12-17)7(16)10-4-3-9-6(15)11-5(4)14/h3H,1-2H2,(H,10,

InchiKey: HHGFJUCVFZPIRF-UHFFFAOYSA-N

Formula: C7H8FN5O4

SMILES: O=NN(CCF)C(=O)Nc1c[nH]c(=O)[nH]c1=O

Mol. weight [g/mol]: 245.17

CAS: 116277-64-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.04		Crippen Method
logp	-1.416		Crippen Method
mcvol	152.280	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116277646&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