Urea, 1-(2-fluoroethyl)-1-nitroso-3-(tetrahydro-2h-thiopy S,S-dioxide

Inchi: InChI=1S/C8H14FN3O4S/c9-3-4-12(11-14)8(13)10-7-1-5-17(15,16)6-2-7/h7H,1-6H2,(H,1

InchiKey: LKCXGNNLVAZPIG-UHFFFAOYSA-N

Formula: C8H14FN3O4S

SMILES: O=NN(CCF)C(=O)NC1CCS(=O)(=O)CC1

Mol. weight [g/mol]: 267.28

CAS: 32319-89-4

Physical Properties

Property code	Value	Unit	Source
hf	-959.97	kJ/mol	Joback Method
hvap	74.97	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	0.226		Crippen Method
mcvol	175.660	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	607.97	K	Joback Method
tc	794.30	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C32319894&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf: Enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature