

Urea, 1-(2-fluoroethyl)-1-nitroso-3-(tetrahydro-2h-thiopyran-2-ylidene)- 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: LKCXGNLVAZPIG-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
mvol	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/ci9903071>
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

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