Urea, 1-(2-fluoroethyl)-3-nitro-

Inchi: InChI=1S/C3H6FN3O3/c4-1-2-5-3(8)6-7(9)10/h1-2H2,(H2,5,6,8)
InchiKey: XAOCRUPQPXSJEN-UHFFFAOYSA-N
Formula: C3H6FN3O3
SMILES: O=C(NCCF)N[N+](=O)[O-]
Mol. weight [g/mol]: 151.10
CAS: 33021-92-0

Physical Properties

Property code	Value	Unit	Source
gf	-135.02	kJ/mol	Joback Method
hf	-317.76	kJ/mol	Joback Method
hfus	29.76	kJ/mol	Joback Method
hvap	57.66	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	-0.553		Crippen Method
mcvol	93.850	ml/mol	McGowan Method
pc	4756.24	kPa	Joback Method
tb	573.36	K	Joback Method
tc	784.33	K	Joback Method
tf	423.02	K	Joback Method
vc	0.380	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.19	J/mol×K	573.36	Joback Method
cpg	233.91	J/mol×K	608.52	Joback Method
cpg	241.14	J/mol×K	643.68	Joback Method
cpg	247.89	J/mol×K	678.85	Joback Method
cpg	254.18	J/mol×K	714.01	Joback Method
cpg	260.02	J/mol×K	749.17	Joback Method
cpg	265.44	J/mol×K	784.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33021920&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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume