

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

Inchi:	InChI=1S/C4H9FN2O/c1-6-4(8)7-3-2-5/h2-3H2,1H3,(H2,6,7,8)
InchiKey:	MFZXOMNMWJPMMG-UHFFFAOYSA-N
Formula:	C4H9FN2O
SMILES:	CNC(=O)NCCF
Mol. weight [g/mol]:	120.13
CAS:	13907-91-0

Physical Properties

Property code	Value	Unit	Source
gf	-162.15	kJ/mol	Joback Method
hf	-327.64	kJ/mol	Joback Method
hfus	20.99	kJ/mol	Joback Method
hvap	43.30	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	-0.115		Crippen Method
mcvol	90.520	ml/mol	McGowan Method
pc	4119.70	kPa	Joback Method
tb	444.40	K	Joback Method
tc	623.46	K	Joback Method
tf	290.68	K	Joback Method
vc	0.353	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.10	J/mol×K	444.40	Joback Method
cpg	197.72	J/mol×K	474.24	Joback Method
cpg	205.97	J/mol×K	504.09	Joback Method
cpg	213.85	J/mol×K	533.93	Joback Method
cpg	221.36	J/mol×K	563.77	Joback Method
cpg	228.53	J/mol×K	593.61	Joback Method
cpg	235.35	J/mol×K	623.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13907910&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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

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