

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

Inchi:	InChI=1S/C9H11FN2O/c10-6-7-11-9(13)12-8-4-2-1-3-5-8/h1-5H,6-7H2,(H2,11,12,13)
InchiKey:	OFIOVEVMZIFQLI-UHFFFAOYSA-N
Formula:	C9H11FN2O
SMILES:	O=C(NCCF)Nc1ccccc1
Mol. weight [g/mol]:	182.19
CAS:	331-07-7

Physical Properties

Property code	Value	Unit	Source
gf	-7.64	kJ/mol	Joback Method
hf	-194.31	kJ/mol	Joback Method
hfus	27.98	kJ/mol	Joback Method
hvap	56.70	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	1.778		Crippen Method
mvol	137.210	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
tb	585.48	K	Joback Method
tc	793.68	K	Joback Method
tf	373.45	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.18	J/molxK	585.48	Joback Method
cpg	345.47	J/molxK	620.18	Joback Method
cpg	356.95	J/molxK	654.88	Joback Method
cpg	367.66	J/molxK	689.58	Joback Method
cpg	377.64	J/molxK	724.28	Joback Method
cpg	386.92	J/molxK	758.98	Joback Method
cpg	395.54	J/molxK	793.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C331077&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

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
mccvol:	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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