

Urea, 3-(2-chloroethyl)-1,1-dimethyl-

Inchi:	InChI=1S/C5H11CIN2O/c1-8(2)5(9)7-4-3-6/h3-4H2,1-2H3,(H,7,9)
InchiKey:	VMJXYAOXDSCSUBQ-UHFFFAOYSA-N
Formula:	C5H11CIN2O
SMILES:	CN(C)C(=O)NCCCI
Mol. weight [g/mol]:	150.61
CAS:	71162-62-4

Physical Properties

Property code	Value	Unit	Source
gf	50.54	kJ/mol	Joback Method
hf	-153.85	kJ/mol	Joback Method
hfus	22.62	kJ/mol	Joback Method
hvap	46.33	kJ/mol	Joback Method
log10ws	-0.58		Crippen Method
logp	0.496		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	467.71	K	Joback Method
tc	655.63	K	Joback Method
tf	311.09	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.23	J/molxK	467.71	Joback Method
cpg	244.50	J/molxK	499.03	Joback Method
cpg	254.24	J/molxK	530.35	Joback Method
cpg	263.47	J/molxK	561.67	Joback Method
cpg	272.22	J/molxK	592.99	Joback Method
cpg	280.49	J/molxK	624.31	Joback Method
cpg	288.31	J/molxK	655.63	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71162624&Units=SI

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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