

Urea, 3-(hydroxymethyl)-1,1-dimethyl-

Inchi:	InChI=1S/C4H10N2O2/c1-6(2)4(8)5-3-7/h7H,3H2,1-2H3,(H,5,8)
InchiKey:	GNIMYRNRLPAMNV-UHFFFAOYSA-N
Formula:	C4H10N2O2
SMILES:	CN(C)C(=O)NCO
Mol. weight [g/mol]:	118.13
CAS:	17660-99-0

Physical Properties

Property code	Value	Unit	Source
gf	-82.77	kJ/mol	Joback Method
hf	-269.70	kJ/mol	Joback Method
hfus	19.92	kJ/mol	Joback Method
hvap	56.40	kJ/mol	Joback Method
log10ws	0.23		Crippen Method
logp	-0.793		Crippen Method
mcvol	94.620	ml/mol	McGowan Method
pc	4849.43	kPa	Joback Method
tb	499.58	K	Joback Method
tc	674.99	K	Joback Method
tf	330.72	K	Joback Method
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.81	J/mol×K	499.58	Joback Method
cpg	222.00	J/mol×K	528.81	Joback Method
cpg	229.80	J/mol×K	558.05	Joback Method
cpg	237.22	J/mol×K	587.28	Joback Method
cpg	244.26	J/mol×K	616.52	Joback Method
cpg	250.95	J/mol×K	645.75	Joback Method
cpg	257.29	J/mol×K	674.99	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17660990&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
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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