Urea, 1,1-bis(2-hydroxyethyl)-3-methyl-

Inchi: InChI=1S/C6H14N2O3/c1-7-6(11)8(2-4-9)3-5-10/h9-10H,2-5H2,1H3,(H,7,11)
InchiKey: VEEUFWDGCHUMFT-UHFFFAOYSA-N
Formula: C6H14N2O3
SMILES: CNC(=O)N(CCO)CCO
Mol. weight [g/mol]: 162.19
CAS: 37437-17-5

Physical Properties

Property code	Value	Unit	Source
gf	-202.75	kJ/mol	Joback Method
hf	-463.21	kJ/mol	Joback Method
hfus	29.19	kJ/mol	Joback Method
hvap	77.53	kJ/mol	Joback Method
log10ws	0.63		Crippen Method
logp	-1.388		Crippen Method
mcvol	128.670	ml/mol	McGowan Method
pc	4238.55	kPa	Joback Method
tb	637.52	K	Joback Method
tc	805.82	K	Joback Method
tf	414.08	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.50	J/mol×K	637.52	Joback Method
cpg	356.07	J/mol×K	665.57	Joback Method
cpg	364.23	J/mol×K	693.62	Joback Method
cpg	371.98	J/mol×K	721.67	Joback Method
cpg	379.33	J/mol×K	749.72	Joback Method
cpg	386.31	J/mol×K	777.77	Joback Method
cpg	392.93	J/mol×K	805.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37437175&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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