bis(hydroxymethyl)urea

Inchi: InChI=1S/C3H8N2O3/c4-3(8)5(1-6)2-7/h6-7H,1-2H2,(H2,4,8)
InchiKey: QAGFPFWZCJWYRP-UHFFFAOYSA-N
Formula: C3H8N2O3
SMILES: NC(=O)N(CO)CO
Mol. weight [g/mol]: 120.11
CAS: 25155-29-7

Physical Properties

Property code	Value	Unit	Source
chs	-1606.80	kJ/mol	NIST Webbook
gf	-250.95	kJ/mol	Joback Method
hf	-420.97	kJ/mol	Joback Method
hfs	-717.05	kJ/mol	NIST Webbook
hfus	21.52	kJ/mol	Joback Method
hvap	75.06	kJ/mol	Joback Method
log10ws	0.65		Crippen Method
logp	-1.733		Crippen Method
mcvol	86.400	ml/mol	McGowan Method
pc	6898.38	kPa	Joback Method
tb	591.24	K	Joback Method
tc	768.26	K	Joback Method
tf	410.87	K	Joback Method
vc	0.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.43	J/mol×K	591.24	Joback Method
cpg	223.25	J/mol×K	620.74	Joback Method
cpg	228.76	J/mol×K	650.25	Joback Method
cpg	233.97	J/mol×K	679.75	Joback Method
cpg	238.88	J/mol×K	709.25	Joback Method
cpg	243.52	J/mol×K	738.75	Joback Method
cpg	247.89	J/mol×K	768.26	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=C25155297&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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