Iminodiacetic acid

Other names:	2,2'-Iminodiacetic acid Acetic acid, 2,2'-iminobis- Acetic acid, iminodi- Aminodiacetic acid Bis(carboxymethyl)amine Diglycin Diglycocoll Diglycollamic acid Glycine, N-(carboxymethyl)- Hampshire IDA IDA (chelating agent) IMDA Iminobis(acetic acid) Iminodiethanoic acid N-(carboxymethyl)glycine NSC 18467 USAF DO-55 diglycine
Inchi:	InChI=1S/C4H7NO4/c6-3(7)1-5-2-4(8)9/h5H,1-2H2,(H,6,7)(H,8,9)
InchiKey:	NBZBKCUXIYYUSX-UHFFFAOYSA-N
Formula:	C4H7NO4
SMILES:	O=C(O)CNCC(=O)O
Mol. weight [g/mol]:	133.10
CAS:	142-73-4

Physical Properties

Property code	Value	Unit	Source
gf	-459.29	kJ/mol	Joback Method
hf	-602.04	kJ/mol	Joback Method
hfus	22.59	kJ/mol	Joback Method
hvap	77.78	kJ/mol	Joback Method
log10ws	1.12		Crippen Method
logp	-1.255		Crippen Method
mcvol	92.080	ml/mol	McGowan Method
pc	6113.06	kPa	Joback Method
tb	633.19	K	Joback Method

tc	811.44	K	Joback Method
tf	409.00	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.93	J/mol×K	633.19	Joback Method
cpg	233.53	J/mol×K	662.90	Joback Method
cpg	238.83	J/mol×K	692.61	Joback Method
cpg	243.84	J/mol×K	722.32	Joback Method
cpg	248.57	J/mol×K	752.03	Joback Method
cpg	253.02	J/mol×K	781.73	Joback Method
cpg	257.20	J/mol×K	811.44	Joback Method

Sources

Enthalpy of dilution and volumetric properties of N-glycylglycine in aqueous xylitol solutions at T = 288.15 K:	https://www.doi.org/10.1016/j.jct.2011.02.005
Volumetric approach to the interaction of diglycine in aqueous solutions of sulpha drugs at T = 288.15 to 308.15 K:	https://www.doi.org/10.1016/j.fluid.2012.08.001
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Densities of aqueous solutions containing model compounds of amino acids and ionic salts at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2006.11.014
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C142734&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Ammonium based ionic liquids act as compatible solvents for glycine peptides:	https://www.doi.org/10.1016/j.jct.2012.07.009
Thermodynamic contributions of peptide backbone unit from water to biocompatible ionic liquids at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2011.09.017
Interaction of some hydrophobic amino acids, peptides, and protein with aqueous 3-chloro-1,2-propanediol and 3-chloro-1-propanol: Biophysical studies:	https://www.doi.org/10.1016/j.jct.2010.11.015
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume