Glycine, N-(carboxymethyl)-

Other names:	2,2'-Iminodiacetic acid
	Acetic acid, 2,2'-iminobis-
	Acetic acid, iminodi-
	Aminodiacetic acid
	Bis(carboxymethyl)amine
	Diglycin
	Diglycocoll
	Diglycollamic acid
	Hampshire
	IDA
	IDA (chelating agent)
	IMDA
	Iminobis(acetic acid)
	Iminodiethanoic acid
	N-(carboxymethyl)glycine
	NSC 18467
	USAF DO-55
	diglycine
	iminodiacetic acid
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

Physical Properties

Property code	Value	Unit	Source
chs	-1641.80 ± 1.20	kJ/mol	NIST Webbook
hf	-742.77	kJ/mol	Cheméo Relay (1.0)
hfs	-932.60 ± 1.30	kJ/mol	NIST Webbook
hfus	22.59	kJ/mol	Joback Method
hvap	97.55	kJ/mol	Cheméo Relay (1.0)
ie	8.92	eV	Cheméo Relay (1.0)
log10ws	0.32		Cheméo Relay (1.0)
logp	-1.255		Crippen Method
mcvol	92.080	ml/mol	McGowan Method
pc	6113.06	kPa	Joback Method

tb	523.76	K	Cheméo Relay (1.0)
tf	458.08	K	Cheméo Relay (1.0)

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 = 298.15 K:	https://www.doi.org/10.1016/j.jct.2011.02.005
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Ammonium based ionic liquids act as compatible solvents for glycine peptides:	https://www.doi.org/10.1016/j.jct.2012.07.009
Transfer Enthalpies of Amino Acids and Glycine Peptides from Water to Aqueous Solutions of Sugar Alcohol at 298.15 K:	https://www.doi.org/10.1021/je800615s
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C142734&Units=SI
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Interaction of some hydrophobic amino acids, peptides, and protein with aqueous 1,2-propanediol and 1-propanol: Biophysical Studies:	https://www.doi.org/10.1016/j.jct.2010.11.015
Transfer Enthalpies of Amino Acids and Glycine Peptides from Water to Aqueous Solutions of Trimethylamine N-Oxide at 298.15 K:	https://www.doi.org/10.1016/j.tca.2014.04.013
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
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

Legend

chs: Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
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
tf:	Normal melting (fusion) point

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