N-Glycylglycine

Other names:	2-(aminoacetamido)acetic acid Diglycine Glycine dipeptide Glycine, N-glycyl- N-(2-aminoacetyl)-2-aminoethanoic acid glycylglycine
Inchi:	InChI=1S/C4H8N2O3/c5-1-3(7)6-2-4(8)9/h1-2,5H2,(H,6,7)(H,8,9)
InchiKey:	YMAWOPBAYDPSLA-UHFFFAOYSA-N
Formula:	C4H8N2O3
SMILES:	NCC(=O)NCC(=O)O
Mol. weight [g/mol]:	132.12
CAS:	556-50-3

Physical Properties

Property code	Value	Unit	Source
basg	882.00	kJ/mol	NIST Webbook
chs	-1978.00	kJ/mol	NIST Webbook
chs	-1969.70 ± 1.30	kJ/mol	NIST Webbook
chs	-1969.70 ± 0.54	kJ/mol	NIST Webbook
chs	-1974.00	kJ/mol	NIST Webbook
gf	-256.02	kJ/mol	Joback Method
hf	-416.02	kJ/mol	Joback Method
hfs	-747.68 ± 0.63	kJ/mol	NIST Webbook
hfs	-747.70 ± 1.30	kJ/mol	NIST Webbook
hfus	23.70	kJ/mol	Joback Method
hvap	71.75	kJ/mol	Joback Method
log10ws	1.01		Crippen Method
logp	-1.854		Crippen Method
mcvol	96.190	ml/mol	McGowan Method
pc	5791.74	kPa	Joback Method
ss	180.30	J/mol×K	NIST Webbook
ss	190.00	J/mol×K	NIST Webbook
tb	613.54	K	Joback Method
tc	808.54	K	Joback Method
tf	431.44	K	Joback Method
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.88	J/mol×K	678.54	Joback Method
cpg	256.87	J/mol×K	711.04	Joback Method
cpg	262.50	J/mol×K	743.54	Joback Method
cpg	267.77	J/mol×K	776.04	Joback Method
cpg	237.76	J/mol×K	613.54	Joback Method
cpg	244.51	J/mol×K	646.04	Joback Method
cpg	272.70	J/mol×K	808.54	Joback Method
cps	149.00	J/mol×K	298.00	NIST Webbook
cps	149.00	J/mol×K	298.00	NIST Webbook
cps	163.97	J/mol×K	298.15	NIST Webbook
cps	161.80	J/mol×K	293.90	NIST Webbook

Sources

Volumetric, conductometric and fluorescence probe studies of interactions between glycyl dipeptides and sodium carbonate in aqueous media.	https://www.doi.org/10.1016/j.jct.2012.01.024
Transfer Partial Molar Isentropic Compressibilities of Glycine, Glycylglycine, and Glycylglycine in Aqueous Solutions at (298.15, 303.15, 313.15, and 323.15) K:	https://www.doi.org/10.1007/s10765-013-1432-0
Volumetric, ultrasonic, and UV absorption studies on solute−solvent interactions in aqueous L-alanine/L-glutamine/glycylglycine from water to 0.512 mol·kg−1 aqueous K_2SO_4 solutions at different temperatures.	https://www.doi.org/10.1016/j.tca.2014.07.025
Physicochemical Behavior of Some Amino Acids/Dipeptides in Aqueous Mixtures of Glycine and its Dipeptide in Aqueous Solutions at T = (298.15-318.15) K:	https://www.doi.org/10.1007/s10765-010-0742-8
NIST Webbook, Glycylglycine, aqueous solution, molality=0.512 mol·kg-1	http://webbook.nist.gov/cgi/cbook.cgi?ID=C556503&Units=SI
Effect of Temperature on the Interactions of Glycyl Dipeptides with Sodium Dodecyl Sulfate in Aqueous Solution: A Volumetric, Conductometric, and Fluorescence Probe Study.	https://www.doi.org/10.1021/je100068y
Joback Method	https://en.wikipedia.org/wiki/Joback_method
Transfer Partial Molar Volumes of L-Alanine/L-Glutamine/Glycylglycine from Water to 0.512 mol/kg Aqueous K_2SO_4 Solutions at (298.15 to 323.15) K:	https://www.doi.org/10.1021/je300083m
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Interactions of amino acids and peptides with the drug chloramphenicol with Glycylglycine in Aqueous Solutions at T = (298.15-318.15) K:	https://www.doi.org/10.1016/j.jct.2012.05.009
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Effect of tetraalkylammonium bromides on the volumetric properties of glycine, L-alanine, and glycylglycine at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2003.09.008
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Effects of Concentration and Temperature Interactions in (L-Alanine/ L-Threonine/ Glycylglycine + Aqueous Glucose / Aqueous Sucrose) Systems: Insights from Viscosity Measurements.	https://www.doi.org/10.1016/j.tca.2013.11.006
Crippen Method	https://www.chemeo.com/doc/models/crippen_log10ws
Interactions of Some Glycyl Dipeptides with Sodium Butyrate in Aqueous Solutions at 298.15 K: Volume and Conductometric Study.	https://www.doi.org/10.1021/je800713c
Interactions in (glycylglycine + 1M aqueous glucose) and (glycylglycine + 1M aqueous sucrose) systems at (298.15 to 323.15) K:	https://www.doi.org/10.1016/j.jct.2005.04.012
	https://www.doi.org/10.1016/j.tca.2011.03.024

Densities, partial molar volumes at infinite dilution, side chain partial molar volumes and transfer volumes of Acid-Tetrapeptan(Glycylglycine+2 M Urea)+Water Ternary Mixtures at T = 298.15 K:	https://www.doi.org/10.1021/je100703r
Viscosities of L-Histidine/L-Glutamic Acid/L-Tryptophan/Glycylglycine+2 M Urea+Water Ternary Mixtures at T = 298.15 K:	https://www.doi.org/10.1007/s10765-011-0996-9
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Volumetric and viscometric studies of interactions of L-alanine, DL-serine, DL-threonine, L-histidine, glycine, and glycylglycine in water, sodium amino acid and alkyl sulfate in aqueous solutions at T=298.15 K:	https://www.doi.org/10.1016/j.jct.2005.03.015
Counteracting effects of trimethylamine N-oxide and betaine on the drug domiphen bromide in aqueous solutions analyzed by volumetric and UV-Vis spectroscopy:	https://www.doi.org/10.1016/j.jct.2016.06.018
Ultrasonic velocities, densities, and viscosities of glycylglycine and CoCl2 in aqueous and aqueous ethanol systems at different temperatures:	https://www.doi.org/10.1016/j.tca.2009.02.017
Behavior at T= 298.15 K of 2-[(2-Aminoacetyl)amino]acetic Acid, glycine dipeptides with aqueous sodium acetate and sodium chloride solutions:	https://www.doi.org/10.1016/j.jct.2010.01.010
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Effect of temperature on the interactions of glycyl dipeptides with aqueous solutions of tetraethylammonium bromide and sodium chloride:	https://www.doi.org/10.1016/j.jct.2011.12.029
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Legend

basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume

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