N-(N-Glycylglycyl)glycine

Other names:	Diglycylglycine
	Glycine, N-(N-glycylglycyl)-
	Glycylglycylglycine
	Triglycine
Inchi:	InChI=1S/C6H11N3O4/c7-1-4(10)8-2-5(11)9-3-6(12)13/h1-3,7H2,(H,8,10)(H,9,11)(H,12,1
InchiKey:	XKUKSGPZAADMRA-UHFFFAOYSA-N
Formula:	C6H11N3O4
SMILES:	NCC(O)=NCC(O)=NCC(=O)O
Mol. weight [g/mol]:	189.17
CAS:	556-33-2

Physical Properties

Property code	Value	Unit	Source
hf	-557.79	kJ/mol	Joback Method
hvap	103.16	kJ/mol	Joback Method
log10ws	1.17		Crippen Method
logp	-1.057		Crippen Method
mcvol	135.920	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
tb	892.74	K	Joback Method
tc	1098.97	K	Joback Method

Sources

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
Thermodynamics of the interactions of some amino acids and peptides with dodecyltrimethylammonium bromide and tetradecyltrimethylammonium bromide:	https://www.doi.org/10.1016/j.jct.2013.11.001
Interaction of some hydrophobic amino acids, peptides, and protein with cosolutes. 3-chloro-1,2-propanediol and 3-chloro-1-propanol: Biophysical studies:	https://www.doi.org/10.1016/j.jct.2010.11.015
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Partial molar volumes, expansibilities and compressibilities of glyglylglycine in aqueous sucrose and fructose solutions between 288.15 to 308.15 K:	https://www.doi.org/10.1016/j.tca.2010.11.013
Interactions of some amino acids and glycine peptides with aqueous sodium dodecyl sulfate and cetyltrimethylammonium bromide at T = 298.15 K: a volumetric approach:	https://www.doi.org/10.1016/j.jct.2003.09.010
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C556332&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Interactions of tripeptide with glucose in aqueous solutions at various temperatures: A volumetric and ultrasonic study:	https://www.doi.org/10.1016/j.tca.2010.05.016

Thermodynamic properties of peptide solutions 20. Partial molar volumes and isothermal compressions for some tripeptides of sequence GlyXGly (X = Ala, Leu, Asn, Thr, Ethionin) in aqueous solutions at T = 298.15 K and p = 0.1 MPa	https://www.doi.org/10.1016/j.jct.2016.03.032
Interactions of some short peptides with the osmolyte trimethylamine N-oxide: an application of McGowan's molecular surface model	https://www.doi.org/10.1016/j.jct.2011.12.029
Studies on the interactions of diglycine and triglycine with polyethylene glycol 200 in aqueous solutions by density and ultrasound speed measurements: Effect of temperature	https://www.doi.org/10.1016/j.jct.2012.10.018
Interactions of the drug pentoxifylline in aqueous solutions of L-valine and its peptides at various temperatures: A volumetric approach	https://www.doi.org/10.1016/j.jct.2012.05.009
Enthalpic Interaction Coefficients of N-(N- Glycylglycyl)glycine in Aqueous Sodium Chloride and Potassium Chloride Solutions at 298.15 K: Interactions of urea with zwitterionic glycine peptides:	https://www.doi.org/10.1021/je0600754
Oligopeptides in Aqueous Solutions. Enthalpic Interaction Coefficients of N-(N- Glycylglycyl)glycine in Aqueous Sodium Chloride and Potassium Chloride Solutions at 298.15 K: Counteracting effects of trimethylamine N-oxide and betaine on the McGowan Method:	https://www.doi.org/10.1021/je900849b
	https://www.doi.org/10.1016/j.tca.2009.02.017
	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation 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