

Glycylglycylglycylglycine

Other names:	Glycine, N-[N-(N-glycylglycyl)glycyl]- N-[N-(N-glycylglycyl)glycyl]glycine tetraglycine
Inchi:	InChI=1S/C8H14N4O5/c9-1-5(13)10-2-6(14)11-3-7(15)12-4-8(16)17/h1-4,9H2,(H,10,13)
InchiKey:	QMOQBVOBWWNSNO-UHFFFAOYSA-N
Formula:	C8H14N4O5
SMILES:	NCC(=O)NCC(=O)NCC(=O)NCC(=O)O
Mol. weight [g/mol]:	246.22
CAS:	637-84-3

Physical Properties

Property code	Value	Unit	Source
affp	973.80	kJ/mol	NIST Webbook
basg	928.20	kJ/mol	NIST Webbook
chs	-3965.00 ± 3.20	kJ/mol	NIST Webbook
gf	-301.40	kJ/mol	Joback Method
hf	-616.80	kJ/mol	Joback Method
hfus	47.45	kJ/mol	Joback Method
hvap	107.01	kJ/mol	Joback Method
log10ws	1.40		Crippen Method
logp	-3.622		Crippen Method
mcvol	175.650	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
tb	913.14	K	Joback Method
tc	1124.30	K	Joback Method
tf	681.70	K	Joback Method
vc	0.660	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.18	J/mol×K	913.14	Joback Method
cpg	544.26	J/mol×K	948.33	Joback Method
cpg	550.67	J/mol×K	983.53	Joback Method

cpg	556.43	J/molxK	1018.72	Joback Method
cpg	561.58	J/molxK	1053.92	Joback Method
cpg	566.13	J/molxK	1089.11	Joback Method
cpg	570.11	J/molxK	1124.30	Joback Method

Sources

Densities of aqueous solutions containing model compounds of amino acids and their effects on the N-oxide and betaine on the solubility of Glycylglycylglycine in Aqueous Solutions: Joback Method:	https://www.doi.org/10.1016/j.jct.2006.11.014
Substituted Glycylglycylglycine	https://www.doi.org/10.1016/j.tca.2009.02.017
Substitution of Glycylglycylglycine	https://www.doi.org/10.1021/je0600754
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=C637843&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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

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