Hexaglycine

Other names:	(glycine)6
	glycine, N-[N-[N-[N-(N-glycylglycyl)glycyl]glycyl]glycyl]glycyl]-
Inchi:	InChI=1S/C12H20N6O7/c13-1-7(19)14-2-8(20)15-3-9(21)16-4-10(22)17-5-11(23)18-6-12
InchiKey:	XJFPXLWGZWAWRQ-UHFFFAOYSA-N
Formula:	C12H20N6O7
SMILES:	NCC(=O)NCC(=O)NCC(=O)NCC(=O)NCC(=O)NCC(=O)O
Mol. weight [g/mol]:	360.32
CAS:	3887-13-6

Physical Properties

Property code	Value	Unit	Source
gf	-346.78	kJ/mol	Joback Method
hf	-817.58	kJ/mol	Joback Method
hfus	71.21	kJ/mol	Joback Method
hvap	142.28	kJ/mol	Joback Method
log10ws	1.80		Crippen Method
logp	-5.389		Crippen Method
mcvol	255.110	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
tb	1212.74	K	Joback Method
tc	1504.97	K	Joback Method
tf	931.96	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.33	J/mol×K	1212.74	Joback Method
cpg	850.32	J/mol×K	1261.45	Joback Method
cpg	853.07	J/mol×K	1310.15	Joback Method
cpg	854.67	J/mol×K	1358.86	Joback Method
cpg	855.22	J/mol×K	1407.56	Joback Method
cpg	854.85	J/mol×K	1456.27	Joback Method
cpg	853.63	J/mol×K	1504.97	Joback Method

Sources

Solubilities of Glycine and Its Oligopeptides in Aqueous Solutions:	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=C3887136&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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