Glycyl-L-phenyl alanine

Other names:	Glycylphenylalanine
	L-Phenylalanine, N-glycyl-
	N-glycyl-3-phenylalanine
Inchi:	InChI=1S/C11H14N2O3/c12-7-10(14)13-9(11(15)16)6-8-4-2-1-3-5-8/h1-5,9H,6-7,12H2,(H
InchiKey:	JBCLFWXMTIKCCB-UHFFFAOYSA-N
Formula:	C11H14N2O3
SMILES:	NCC(=O)NC(Cc1ccccc1)C(=O)O
Mol. weight [g/mol]:	222.24
CAS:	3321-03-7

Physical Properties

Property code	Value	Unit	Source
chs	-5645.10 ± 1.80	kJ/mol	NIST Webbook
gf	-87.11	kJ/mol	Joback Method
hf	-329.25	kJ/mol	Joback Method
hfus	32.35	kJ/mol	Joback Method
hvap	89.22	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	-0.243		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
tb	799.94	K	Joback Method
tc	1014.88	K	Joback Method
tf	521.75	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.79	J/mol×K	799.94	Joback Method
cpg	502.59	J/mol×K	835.76	Joback Method
cpg	511.63	J/mol×K	871.59	Joback Method
cpg	519.95	J/mol×K	907.41	Joback Method
cpg	527.59	J/mol×K	943.23	Joback Method

cpg	534.59	J/mol×K	979.06	Joback Method
cpg	541.01	J/mol×K	1014.88	Joback Method

Sources

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=C3321037&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Densities, partial molar volumes at infinite dilution, side chain partial molar volumes and transfer volumes of dipeptides in sucrose and 2,3-butanediol aqueous solutions at T = (283.15–333.15) K:	https://www.doi.org/10.1021/je100703r

Legend

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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