

N-dl-Alanylglycine

Other names:	Glycine, N-DL-alanyl-
Inchi:	InChI=1S/C5H10N2O3/c1-3(6)5(10)7-2-4(8)9/h3H,2,6H2,1H3,(H,7,10)(H,8,9)
InchiKey:	CXISPYVVMQWFLE-UHFFFAOYSA-N
Formula:	C5H10N2O3
SMILES:	CC(N)C(=O)NCC(=O)O
Mol. weight [g/mol]:	146.14
CAS:	1188-01-8

Physical Properties

Property code	Value	Unit	Source
chs	-2618.90 ± 0.84	kJ/mol	NIST Webbook
gf	-250.04	kJ/mol	Joback Method
hf	-441.94	kJ/mol	Joback Method
hfs	-777.39 ± 0.88	kJ/mol	NIST Webbook
hfus	22.77	kJ/mol	Joback Method
hvap	73.58	kJ/mol	Joback Method
log10ws	0.47		Crippen Method
logp	-1.466		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
ss	213.40	J/mol×K	NIST Webbook
tb	635.98	K	Joback Method
tc	832.14	K	Joback Method
tf	427.71	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.45	J/mol×K	799.44	Joback Method
cpg	283.69	J/mol×K	635.98	Joback Method
cpg	291.53	J/mol×K	668.67	Joback Method
cpg	298.92	J/mol×K	701.37	Joback Method
cpg	305.86	J/mol×K	734.06	Joback Method

cpg	312.36	J/mol×K	766.75	Joback Method
cpg	324.14	J/mol×K	832.14	Joback Method
cps	181.79	J/mol×K	296.40	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1188018&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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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