

L-Alanine, N-methyl-

Other names:	Alanine, N-methyl-, L- «alpha»-(Methylamino)propionic acid L-N-Methylalanine N-Methyl-L-alanine N-Methylalanine
Inchi:	InChI=1S/C4H9NO2/c1-3(5-2)4(6)7/h3,5H,1-2H3,(H,6,7)/t3-/m1/s1
InchiKey:	GDFAOVXKHJXLEI-GSVOUGTGSA-N
Formula:	C4H9NO2
SMILES:	CNC(C)C(=O)O
Mol. weight [g/mol]:	103.12
CAS:	3913-67-5

Physical Properties

Property code	Value	Unit	Source
gf	-195.99	kJ/mol	Joback Method
hf	-342.51	kJ/mol	Joback Method
hfus	13.38	kJ/mol	Joback Method
hvap	53.97	kJ/mol	Joback Method
log10ws	0.10		Crippen Method
logp	-0.321		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
pc	4917.69	kPa	Joback Method
tb	486.70	K	Joback Method
tc	667.62	K	Joback Method
tf	283.25	K	Joback Method
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.19	J/molxK	486.70	Joback Method
cpg	190.71	J/molxK	516.85	Joback Method
cpg	197.89	J/molxK	547.01	Joback Method
cpg	204.75	J/molxK	577.16	Joback Method

cpg	211.29	J/mol×K	607.31	Joback Method
cpg	217.51	J/mol×K	637.46	Joback Method
cpg	223.44	J/mol×K	667.62	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=C3913675&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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