

norvaline

Other names:	(S)-2-aminopentanoic acid L-.alpha.-aminovaleric acid L-norvaline
Inchi:	InChI=1S/C5H11NO2/c1-2-3-4(6)5(7)8/h4H,2-3,6H2,1H3,(H,7,8)/t4-/m1/s1
InchiKey:	SNDPXSYFESPGGJ-SCSAIBSYSA-N
Formula:	C5H11NO2
SMILES:	CCCC(N)C(=O)O
Mol. weight [g/mol]:	117.15
CAS:	6600-40-4

Physical Properties

Property code	Value	Unit	Source
gf	-210.51	kJ/mol	Joback Method
hf	-382.83	kJ/mol	Joback Method
hfus	16.07	kJ/mol	Joback Method
hvap	60.40	kJ/mol	Joback Method
ie	8.53	eV	NIST Webbook
log10ws	-0.56		Crippen Method
logp	0.198		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	4577.74	kPa	Joback Method
tb	531.94	K	Joback Method
tc	719.19	K	Joback Method
tf	325.12	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.00	J/mol×K	531.94	Joback Method
cpg	240.44	J/mol×K	563.15	Joback Method
cpg	248.49	J/mol×K	594.36	Joback Method
cpg	256.14	J/mol×K	625.57	Joback Method
cpg	263.41	J/mol×K	656.78	Joback Method

cpg	270.32	J/mol×K	687.99	Joback Method
cpg	276.87	J/mol×K	719.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6600404&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Ternary phase diagram and the formation mechanism of two distinct solubility regions of amino acid systems:	https://www.doi.org/10.1016/j.jct.2017.12.010
Joback Method	https://en.wikipedia.org/wiki/Joback_method
L-Valine/L-norvaline and L-valine/L-alanine:	

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
ie:	Ionization energy
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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