Valine

Other names:	L-Valine
	Valine, L-
	Butanoic acid, 2-amino-3-methyl-
	Butanoic acid, 2-amino-3-methyl-, (S)-
	L-(+)-«alpha»-Aminoisovaleric acid
	2-Amino-3-methylbutanoic acid
	2-Amino-3-methylbutyric acid
	L-iso-C3H7CH(NH2)COOH
	(S)-2-Amino-3-methylbutanoic acid
	(S)-2-Amino-3-methylbutyric acid
	(S)-Valine
	NSC 76038
Inchi:	InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m1/s1
InchiKey:	KZSNJWFQEVHDMF-SCSAIBSYSA-N
Formula:	C5H11NO2
SMILES:	CC(C)C(N)C(=O)O
Mol. weight [g/mol]:	117.15
CAS:	72-18-4

Physical Properties

Property code	Value	Unit	Source
affp	910.60	kJ/mol	NIST Webbook
basg	873.00 ± 3.00	kJ/mol	NIST Webbook
basg	876.70	kJ/mol	NIST Webbook
chs	-2910.70 ± 1.90	kJ/mol	NIST Webbook
chs	-2920.10 ± 0.54	kJ/mol	NIST Webbook
gf	-212.95	kJ/mol	Joback Method
hf	-388.11	kJ/mol	Joback Method
hfs	-618.00	kJ/mol	NIST Webbook
hfs	-628.90 ± 1.90	kJ/mol	NIST Webbook
hfus	12.54	kJ/mol	Joback Method
hvap	60.01	kJ/mol	Joback Method
ie	8.71	eV	NIST Webbook
log10ws	-0.32		Crippen Method
logp	0.054		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	4627.70	kPa	Joback Method

ss	178.87	J/mol×K	NIST Webbook
tb	531.50	K	Joback Method
tc	722.61	K	Joback Method
tf	310.12	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.58	J/mol×K	658.91	Joback Method
cpg	271.63	J/mol×K	690.76	Joback Method
cpg	232.36	J/mol×K	531.50	Joback Method
cpg	241.05	J/mol×K	563.35	Joback Method
cpg	249.30	J/mol×K	595.20	Joback Method
cpg	257.14	J/mol×K	627.06	Joback Method
cpg	278.30	J/mol×K	722.61	Joback Method
cps	168.50	J/mol×K	298.15	NIST Webbook
cps	168.82	J/mol×K	298.15	NIST Webbook
hsubt	163.00 ± 0.80	kJ/mol	455.00	NIST Webbook
hsubt	163.00 ± 8.00	kJ/mol	455.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72184&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

affp: Proton affinity
basg: Gas basicity
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
hsubt:	Enthalpy of sublimation at a given temperature
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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume