DL-Valine

Other names:	(RS)-valine
	2-Amino-3-methylbutanoic acid, DL-
	DL-2-amino-3-methylbutanoic acid
	DL-2-amino-3-methylbutyric acid
	DL-2-aminoisobutyric acid
	DL-Val
	DL-«alpha»-Aminoisovaleric acid
	NSC 9755
	Valine
	Valine, DL-
	butanoic acid, 3-amino-2-methyl-, (RS)-
Inchi:	InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)
InchiKey:	KZSNJWFQEVHDMF-UHFFFAOYSA-N
Formula:	C5H11NO2
SMILES:	CC(C)C(N)C(=O)O
Mol. weight [g/mol]:	117.15
CAS:	516-06-3

Physical Properties

Property code	Value	Unit	Source
chs	-2933.90 ± 0.40	kJ/mol	NIST Webbook
chs	-2910.70 ± 1.90	kJ/mol	NIST Webbook
gf	-212.95	kJ/mol	Joback Method
hf	-388.11	kJ/mol	Joback Method
hfs	-617.00 ± 1.00	kJ/mol	NIST Webbook
hfus	12.54	kJ/mol	Joback Method
hvap	60.01	kJ/mol	Joback Method
log10ws	-0.32		Crippen Method
logp	0.054		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	4627.70	kPa	Joback Method
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	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	264.58	J/mol×K	658.91	Joback Method
cpg	271.63	J/mol×K	690.76	Joback Method
cpg	278.30	J/mol×K	722.61	Joback Method
cps	165.00	J/mol×K	298.00	NIST Webbook
cps	164.50	J/mol×K	298.00	NIST Webbook

Sources

Volumetric and Viscosity Properties of r-Amino Acids and Their Groups in Aqueous Sodium Caprylate Solutions:	https://www.doi.org/10.1021/je0501484
Solubility and Thermodynamics of Solute-Solvent Interactions of Some Amino Acids in Aqueous Sodium Bromide and Potassium Bromide Solutions:	https://www.doi.org/10.1021/acs.jced.7b00647
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Partial Molar Volumes and Viscosities of Some r-Amino Acids in Micellar Solutions of Sodium Caprylate:	https://www.doi.org/10.1021/je049927v
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C516063&Units=SI
Interactions of some ex-amino acids with tetra-n-alkylammonium bromides in aqueous medium at different temperatures:	https://www.doi.org/10.1016/j.jct.2006.08.010
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Volumetric, viscometric, and refractive index behaviour of a-amino acids and their groups? contribution in aqueous D-glucose solution at different temperatures:	https://www.doi.org/10.1016/j.jct.2005.04.011

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume