Serine

Other names:	(R)-(-)-serine (R)-2-amino-3-hydroxypropanoic acid (S)-(-)-Serine (S)-2-Amino-3-hydroxypropanoic acid (S)-Serine 2-Amino-3-hydroxypropanoic acid-, (S)- 2-Amino-3-hydroxypropionic acid 3-Hydroxyalanine D-serine L-(-)-Serine L-Ser L-Serine Propanoic acid, 2-amino-3-hydroxy-, (S)- Serine, L- l-2-Amino-3-hydroxy-propanoic acid l-2-Amino-3-hydroxypropionic acid propanoic acid, 2-amino-3-hydroxy-, (R)- «alpha»-Amino-«beta»-hydroxypropionic acid-, (S)- «beta»-Hydroxyalanine Â«alphaÂ»-Amino-Â«betaÂ»-hydroxypropionic acid-, (S)- Â«betaÂ»-Hydroxyalanine
Inchi:	InChI=1S/C3H7NO3/c4-2(1-5)3(6)7/h2,5H,1,4H2,(H,6,7)/t2-/m1/s1
InchiKey:	MTCFGRXMJLQNBG-UWTATZPHSA-N
Formula:	C3H7NO3
SMILES:	NC(CO)C(=O)O
Mol. weight [g/mol]:	105.09
CAS:	56-45-1

Physical Properties

Property code	Value	Unit	Source
affp	912.50	kJ/mol	NIST Webbook
affp	904.50 ± 4.30	kJ/mol	NIST Webbook
affp	914.60	kJ/mol	NIST Webbook
basg	880.70	kJ/mol	NIST Webbook
basg	870.60 ± 4.30	kJ/mol	NIST Webbook
chs	-1448.21 ± 0.18	kJ/mol	NIST Webbook

gf	-364.17	kJ/mol	Joback Method
hf	-493.78	kJ/mol	Joback Method
hfs	-732.73 ± 0.28	kJ/mol	NIST Webbook
hfus	14.97	kJ/mol	Joback Method
hvap	72.63	kJ/mol	Joback Method
log10ws	-1.14		Aqueous Solubility Prediction Method
logp	-1.609		Crippen Method
mcvol	76.420	ml/mol	McGowan Method
pc	7014.41	kPa	Joback Method
ss	149.16	J/mol×K	NIST Webbook
tb	578.36	K	Joback Method
tc	760.22	K	Joback Method
tf	363.40	K	Joback Method
vc	0.271	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.33	J/mol×K	699.60	Joback Method
cpg	208.59	J/mol×K	729.91	Joback Method
cpg	184.80	J/mol×K	578.36	Joback Method
cpg	190.08	J/mol×K	608.67	Joback Method
cpg	195.08	J/mol×K	638.98	Joback Method
cpg	199.83	J/mol×K	669.29	Joback Method
cpg	212.60	J/mol×K	760.22	Joback Method
cps	138.90	J/mol×K	298.15	NIST Webbook
cps	135.56	J/mol×K	298.15	NIST Webbook

Sources

Thermodynamics of proton dissociations from aqueous serine at temperatures from (278.15 to 393.15) K, molalities from (0.01 up to 1.0) mol Ae kg-1 and at the pressure 0.35 MPa:	https://www.doi.org/10.1016/j.jct.2005.07.019
A thermochemical study of serine stereoisomers:	https://www.doi.org/10.1016/j.tca.2014.08.032
Temperature Dependences and Enthalpic Discrimination of Homochiral Apparent Molal Heat Capacities and Apparent Molal Volumes of Serine, Aspartic Acid, and Glutamic Acid Enantiomers in Pure Water:	https://www.doi.org/10.1021/je500825a
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
serinate:	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56451&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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