2-Amino-3-hydroxypropionic acid

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)- 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)- serine «alpha»-Amino-«beta»-hydroxypropionic acid-, (S)- «beta»-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

Physical Properties

Property code	Value	Unit	Source
hf	-587.51	kJ/mol	Cheméo Relay (1.0)
hfus	14.97	kJ/mol	Joback Method
ie	9.36	eV	Cheméo Relay (1.0)
log10ws	-1.14		Aqueous Solubility Prediction Method
logp	-1.609		Crippen Method
mcvol	76.420	ml/mol	McGowan Method
tf	506.25	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	204.33	J/mol×K	699.60	Joback Method
cpg	208.59	J/mol×K	729.91	Joback Method
cpg	212.60	J/mol×K	760.22	Joback Method

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C302841&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Apparent molar heat capacities and apparent molar volumes of serine, serinium chloride, and sodium serinate:	https://www.doi.org/10.1016/j.tca.2014.08.032
A thermochemical study of serine stereoisomers:	
Cheméo Relay (1.0, beta):	
Temperature Dependences and Enthalpic Discrimination of Homochiral Pairwise Interactions of Six α-Amino Acid Enantiomers in Pure Water:	https://www.doi.org/10.1021/je500825a
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point