

dl-Threonine

Other names:	(.+-.)-threonine 2-amino-3-hydroxybutanoic acid DL-2-amino-3-hydroxybutanoic acid Threonine, DL- threonine
Inchi:	InChI=1S/C4H9NO3/c1-2(6)3(5)4(7)8/h2-3,6H,5H2,1H3,(H,7,8)
InchiKey:	AYFVYJQAPQTCCC-UHFFFAOYSA-N
Formula:	C4H9NO3
SMILES:	CC(O)C(N)C(=O)O
Mol. weight [g/mol]:	119.12
CAS:	80-68-2

Physical Properties

Property code	Value	Unit	Source
chs	-2101.50 ± 0.42	kJ/mol	NIST Webbook
gf	-358.19	kJ/mol	Joback Method
hf	-519.70	kJ/mol	Joback Method
hfus	14.04	kJ/mol	Joback Method
hvap	74.47	kJ/mol	Joback Method
log10ws	0.48		Crippen Method
logp	-1.221		Crippen Method
mcvol	90.510	ml/mol	McGowan Method
pc	6084.49	kPa	Joback Method
tb	600.80	K	Joback Method
tc	784.19	K	Joback Method
tf	359.67	K	Joback Method
vc	0.321	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.46	J/mol×K	600.80	Joback Method
cpg	234.89	J/mol×K	631.37	Joback Method
cpg	240.98	J/mol×K	661.93	Joback Method

cpg	246.76	J/molxK	692.50	Joback Method
cpg	252.22	J/molxK	723.06	Joback Method
cpg	257.38	J/molxK	753.63	Joback Method
cpg	262.25	J/molxK	784.19	Joback Method

Sources

Solubility of Chiral Threonine Species in Water/Ethanol Mixtures:
Crippen Method:

<https://www.doi.org/10.1021/je060053h>

https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C80682&Units=SI>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Thermodynamics of proton dissociations from aqueous threonine and serine at temperatures from (278.15 to 393.15) K, molalities from (0.01 to 1.0) mol kg⁻¹, and at the state (0.101325 MPa): Apparent molar heat capacities and apparent molar volumes of zwitterionic, protonated, and deprotonated amino acids in binary aqueous solutions of L-alanine, DL-serine, DL-threonine, L-histidine, glycine, and glycyglycine in water, NaCl, and DMSO aqueous solutions at T = 298.15 K:

<https://www.doi.org/10.1016/j.jct.2006.05.013>

https://en.wikipedia.org/wiki/Joback_method

<https://www.doi.org/10.1016/j.tca.2013.04.001>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

<https://www.doi.org/10.1016/j.fluid.2007.10.013>

<https://www.doi.org/10.1016/j.jct.2005.03.015>

Legend

chs:	Standard solid enthalpy of combustion
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
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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