

D-Allothreonine

Other names:	Allothreonine, D- D-threonine DL-allothreonine allothreonine l-Allo-threonine
Inchi:	InChI=1S/C4H9NO3/c1-2(6)3(5)4(7)8/h2-3,6H,5H2,1H3,(H,7,8)/t2-,3-/m0/s1
InchiKey:	AYFVYJQAPQTCCC-HRFVKAFMSA-N
Formula:	C4H9NO3
SMILES:	CC(O)C(N)C(=O)O
Mol. weight [g/mol]:	119.12
CAS:	24830-94-2

Physical Properties

Property code	Value	Unit	Source
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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.46	J/molxK	600.80	Joback Method
cpg	234.89	J/molxK	631.37	Joback Method
cpg	240.98	J/molxK	661.93	Joback Method
cpg	246.76	J/molxK	692.50	Joback Method

cpg	252.22	J/mol×K	723.06	Joback Method
cpg	257.38	J/mol×K	753.63	Joback Method
cpg	262.25	J/mol×K	784.19	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Effects of hydroxyl groups on binary diffusion coefficients of -amino acids in aqueous solutions:	https://www.doi.org/10.1016/j.fluid.2007.10.013
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24830942&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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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