

# Taurine

<b>Other names:</b>	2-aminoethanesulfonic acid Aminoethanesulfonic acid Ethanesulfonic acid, 2-amino-O-Due «beta»-Aminoethylsulfonic acid
<b>Inchi:</b>	InChI=1S/C2H7NO3S/c3-1-2-7(4,5)6/h1-3H2,(H,4,5,6)
<b>InchiKey:</b>	XOAAWQZATWQOTB-UHFFFAOYSA-N
<b>Formula:</b>	C2H7NO3S
<b>SMILES:</b>	NCCS(=O)(=O)O
<b>Mol. weight [g/mol]:</b>	125.15
<b>CAS:</b>	107-35-7

## Physical Properties

Property code	Value	Unit	Source
gf	-572.95	kJ/mol	Joback Method
hf	-656.40	kJ/mol	Joback Method
hfus	21.60	kJ/mol	Joback Method
hvap	66.00	kJ/mol	Joback Method
log10ws	0.76		Crippen Method
logp	-1.167		Crippen Method
mcvol	82.980	ml/mol	McGowan Method
pc	8175.04	kPa	Joback Method
ss	154.00	J/mol×K	NIST Webbook
tb	457.65	K	Joback Method
tc	632.73	K	Joback Method
tf	294.94	K	Joback Method
vc	0.322	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.67	J/mol×K	457.65	Joback Method
cpg	177.95	J/mol×K	486.83	Joback Method
cpg	184.00	J/mol×K	516.01	Joback Method

cpg	189.82	J/mol×K	545.19	Joback Method
cpg	195.39	J/mol×K	574.37	Joback Method
cpg	200.71	J/mol×K	603.55	Joback Method
cpg	205.79	J/mol×K	632.73	Joback Method
cps	140.54	J/mol×K	300.30	NIST Webbook

## Sources

**Joback Method:**

[https://en.wikipedia.org/wiki/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=C107357&Units=SI>

**Crippen Method:**

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

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Determination and Correlation of the Solubility for Taurine in Water and Organic Solvent Systems:**

<https://www.doi.org/10.1021/je9009877>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>cps:</b>	Solid phase heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>ss:</b>	Solid phase molar entropy at standard conditions
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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