

Taurine

Other names:	2-aminoethanesulfonic acid Aminoethanesulfonic acid Ethanesulfonic acid, 2-amino- O-Due «beta»-Aminoethylsulfonic acid
Inchi:	InChI=1S/C2H7NO3S/c3-1-2-7(4,5)6/h1-3H2,(H,4,5,6)
InchiKey:	XOAAWQZATWQOTB-UHFFFAOYSA-N
Formula:	C2H7NO3S
SMILES:	NCCS(=O)(=O)O
Mol. weight [g/mol]:	125.15
CAS:	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
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/ci990307l
Crippen Method:	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

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/61-469-4/Taurine.pdf>

Generated by Cheméo on 2025-12-05 15:36:15.237443183 +0000 UTC m=+4697172.767483836.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.