

ETHANESULFONIC ACID, 2-AMINO-

Other names:	2-aminoethanesulfonic acid Aminoethanesulfonic acid O-Due taurine «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

Physical Properties

Property code	Value	Unit	Source
hfus	21.60	kJ/mol	Joback Method
logp	-1.167		Crippen Method
mcvol	82.980	ml/mol	McGowan Method
ss	154.00	J/mol×K	NIST Webbook

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Determination and Correlation of the Solubility for Taurine in Water and Organic Solvent Systems:	https://www.doi.org/10.1021/je9009877
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107357&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ss:	Solid phase molar entropy at standard conditions

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