N,N-Bis(2-hydroxyethyl)-2-aminoethanesulfonic acid

Other names: Ethanesulfonic acid, 2-[bis(2-hydroxyethyl)amino]-
N,N-Bis(hydroxyethyl)-2-aminoethanesulfonic acid
Taurine, N,N-bis(2-hydroxyethyl)-
2-(Bis(2-Hydroxyethyl)amino)ethanesulfonic acid
BES
2-[bis(2-hydroxyethyl)amino]ethanesulphonic acid

Inchi: InChI=1S/C6H15NO5S/c8-4-1-7(2-5-9)3-6-13(10,11)12/h8-9H,1-6H2,(H,10,11,12)

InchiKey: AJTVSSFTXWNIRG-UHFFFAOYSA-N

Formula: C6H15NO5S

SMILES: O=S(=O)(O)CCN(CCO)CCO

Mol. weight [g/mol]: 213.25

CAS: 10191-18-1

Physical Properties

Property code	Value	Unit	Source
gf	-768.58	kJ/mol	Joback Method
hf	-1009.68	kJ/mol	Joback Method
hfus	37.96	kJ/mol	Joback Method
hvap	99.66	kJ/mol	Joback Method
log10ws	1.42		Crippen Method
logp	-1.839		Crippen Method
mcvol	151.080	ml/mol	McGowan Method
pc	5367.04	kPa	Joback Method
tb	673.44	K	Joback Method
tc	832.63	K	Joback Method
tf	410.87	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.60	J/mol×K	673.44	Joback Method
cpg	425.04	J/mol×K	699.97	Joback Method
cpg	433.05	J/mol×K	726.50	Joback Method

cpg	440.63	J/mol×K	753.03	Joback Method
cpg	447.80	J/mol×K	779.56	Joback Method
cpg	454.56	J/mol×K	806.10	Joback Method
cpg	460.91	J/mol×K	832.63	Joback Method

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=C10191181&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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