2,2'-(tert-Butylimino)diethanol

Other names:	2,2'-[(1,1-dimethylethyl)imino]bisethanol
	2,2-(tert-Butylimino)diethanol
	Ethanol, 2,2'-[(1,1-dimethylethyl)imino]bis-
	N-t-Butyldiethanolamine
	N-tert-Butyl-2,2'-iminodiethanol
	N-tert-Butyldiethanolamine
	tert-Butyldiethanolamine
Inchi:	InChI=1S/C8H19NO2/c1-8(2,3)9(4-6-10)5-7-11/h10-11H,4-7H2,1-3H3
InchiKey:	XHJGXOOOMKCJPP-UHFFFAOYSA-N
Formula:	C8H19NO2
SMILES:	CC(C)(C)N(CCO)CCO
Mol. weight [g/mol]:	161.24
CAS:	2160-93-2

Physical Properties

Property code	Value	Unit	Source
gf	-143.54	kJ/mol	Joback Method
hf	-454.13	kJ/mol	Joback Method
hfus	20.26	kJ/mol	Joback Method
hvap	67.51	kJ/mol	Joback Method
log10ws	-0.38		Crippen Method
logp	0.072		Crippen Method
mcvol	145.300	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
tb	576.01	K	Joback Method
tc	738.82	K	Joback Method
tf	336.45	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.68	J/mol×K	576.01	Joback Method
cpg	394.85	J/mol×K	603.15	Joback Method

cpg	405.46	J/mol×K	630.28	Joback Method
cpg	415.56	J/mol×K	657.42	Joback Method
cpg	425.16	J/mol×K	684.55	Joback Method
cpg	434.29	J/mol×K	711.69	Joback Method
cpg	442.98	J/mol×K	738.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	432.50 ± 1.50	K	2.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.31643e+01
Coeff. B	-4.04682e+03
Coeff. C	-7.71800e+01
Temperature range (K), min.	391.45
Temperature range (K), max.	592.51

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2160932&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume