

# 2,2'-(tert-Butylimino)diethanol

<b>Other names:</b>	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
<b>Inchi:</b>	InChI=1S/C8H19NO2/c1-8(2,3)9(4-6-10)5-7-11/h10-11H,4-7H2,1-3H3
<b>InchiKey:</b>	XHJGXOOOMKCJPP-UHFFFAOYSA-N
<b>Formula:</b>	C8H19NO2
<b>SMILES:</b>	CC(C)(C)N(CCO)CCO
<b>Mol. weight [g/mol]:</b>	161.24
<b>CAS:</b>	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	m <sup>3</sup> /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	$\ln(P_{vp}) = A + B/(T + C)$
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

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2160932&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2160932&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>

# Legend

<b>cpg:</b>	Ideal gas 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>hvac:</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>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/62-584-5/2-2-tert-Butylimino-diethanol.pdf>

Generated by Cheméo on 2024-04-09 06:09:32.928355745 +0000 UTC m=+14932221.848933056.

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