

# 2-(Butylamino)ethanethiol

<b>Other names:</b>	Ethanethiol, 2-(butylamino)- 2-N-Butylaminoethanethiol (butylamino)ethanethiol
<b>Inchi:</b>	InChI=1S/C6H15NS/c1-2-3-4-7-5-6-8/h7-8H,2-6H2,1H3
<b>InchiKey:</b>	OUMFAUYLXGTBCX-UHFFFAOYSA-N
<b>Formula:</b>	C6H15NS
<b>SMILES:</b>	CCCCNCCS
<b>Mol. weight [g/mol]:</b>	133.25
<b>CAS:</b>	5842-00-2

## Physical Properties

Property code	Value	Unit	Source
gf	118.42	kJ/mol	Joback Method
hf	-75.22	kJ/mol	Joback Method
hfus	20.44	kJ/mol	Joback Method
hvap	42.12	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.306		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
tb	449.71	K	Joback Method
tc	642.15	K	Joback Method
tf	246.50	K	Joback Method
vc	0.461	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.10	J/mol×K	449.71	Joback Method
cpg	259.25	J/mol×K	481.78	Joback Method
cpg	270.86	J/mol×K	513.86	Joback Method
cpg	281.95	J/mol×K	545.93	Joback Method
cpg	292.53	J/mol×K	578.00	Joback Method
cpg	302.61	J/mol×K	610.08	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	386.70	K	1.30	NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=C5842002&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5842002&amp;Units=SI</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>hvap:</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>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

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