

# Aniline, 2-tert-butyl-n-sec-butyl-

<b>Inchi:</b>	InChI=1S/C14H23N/c1-6-11(2)15-13-10-8-7-9-12(13)14(3,4)5/h7-11,15H,6H2,1-5H3
<b>InchiKey:</b>	WBRFKMQTYCMFKI-UHFFFAOYSA-N
<b>Formula:</b>	C14H23N
<b>SMILES:</b>	CCC(C)Nc1ccccc1C(C)(C)C
<b>Mol. weight [g/mol]:</b>	205.34

## Physical Properties

Property code	Value	Unit	Source
gf	259.57	kJ/mol	Joback Method
hf	-67.79	kJ/mol	Joback Method
hfus	19.83	kJ/mol	Joback Method
hvap	54.45	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	4.194		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
tb	597.88	K	Joback Method
tc	809.14	K	Joback Method
tf	326.56	K	Joback Method
vc	0.730	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.25	J/molxK	597.88	Joback Method
cpg	521.07	J/molxK	633.09	Joback Method
cpg	538.71	J/molxK	668.30	Joback Method
cpg	555.25	J/molxK	703.51	Joback Method
cpg	570.73	J/molxK	738.72	Joback Method
cpg	585.22	J/molxK	773.93	Joback Method
cpg	598.79	J/molxK	809.14	Joback Method

# Sources

<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=B6009272&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009272&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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