

# Aniline, 2-tert-butyl-n-beta-cyanoethyl-

<b>Inchi:</b>	InChI=1S/C13H18N2/c1-13(2,3)11-7-4-5-8-12(11)15-10-6-9-14/h4-5,7-8,15H,6,10H2,1-3
<b>InchiKey:</b>	QHVNKKFGZMLGBM-UHFFFAOYSA-N
<b>Formula:</b>	C13H18N2
<b>SMILES:</b>	CC(C)(C)c1ccccc1NCCC#N
<b>Mol. weight [g/mol]:</b>	202.30

## Physical Properties

Property code	Value	Unit	Source
gf	386.77	kJ/mol	Joback Method
hf	123.01	kJ/mol	Joback Method
hfus	22.27	kJ/mol	Joback Method
hvap	63.09	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.310		Crippen Method
mcvol	181.630	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
tb	677.52	K	Joback Method
tc	901.34	K	Joback Method
tf	395.28	K	Joback Method
vc	0.706	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.34	J/molxK	677.52	Joback Method
cpg	499.97	J/molxK	714.82	Joback Method
cpg	513.58	J/molxK	752.13	Joback Method
cpg	526.25	J/molxK	789.43	Joback Method
cpg	538.04	J/molxK	826.73	Joback Method
cpg	549.02	J/molxK	864.04	Joback Method
cpg	559.26	J/molxK	901.34	Joback Method

# Sources

<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>
<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=B6009280&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009280&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>mccvol:</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

Latest version available from:

<https://www.chemeo.com/cid/83-158-5/Aniline-2-tert-butyl-n-beta-cyanoethyl.pdf>

Generated by Cheméo on 2024-04-23 06:08:16.997451531 +0000 UTC m=+16141745.918028842.

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