

# Aniline, 2-tert-butyl-5-methyl-

<b>Inchi:</b>	InChI=1S/C11H17N/c1-8-5-6-9(10(12)7-8)11(2,3)4/h5-7H,12H2,1-4H3
<b>InchiKey:</b>	FTOZGMHUVVLXHM-UHFFFAOYSA-N
<b>Formula:</b>	C11H17N
<b>SMILES:</b>	<chem>Cc1ccc(C(C)(C)C)c(N)c1</chem>
<b>Mol. weight [g/mol]:</b>	163.26

## Physical Properties

Property code	Value	Unit	Source
gf	204.18	kJ/mol	Joback Method
hf	-31.74	kJ/mol	Joback Method
hfus	15.29	kJ/mol	Joback Method
hvap	53.03	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.875		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
tb	557.02	K	Joback Method
tc	785.11	K	Joback Method
tf	350.87	K	Joback Method
vc	0.561	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.85	J/molxK	557.02	Joback Method
cpg	382.00	J/molxK	595.03	Joback Method
cpg	397.09	J/molxK	633.05	Joback Method
cpg	411.16	J/molxK	671.06	Joback Method
cpg	424.29	J/molxK	709.08	Joback Method
cpg	436.54	J/molxK	747.09	Joback Method
cpg	447.95	J/molxK	785.11	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=B6008465&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008465&amp;Units=SI</a>
<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>

# 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

Latest version available from:

<https://www.chemeo.com/cid/51-215-6/Aniline-2-tert-butyl-5-methyl.pdf>

Generated by Cheméo on 2024-04-20 16:07:21.609152887 +0000 UTC m=+15918490.529730223.

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