

# Aniline, o-tert-butyl-n-methyl-

<b>Inchi:</b>	InChI=1S/C11H17N/c1-11(2,3)9-7-5-6-8-10(9)12-4/h5-8,12H,1-4H3
<b>InchiKey:</b>	DHQJBOWJBHNPIF-UHFFFAOYSA-N
<b>Formula:</b>	C11H17N
<b>SMILES:</b>	CNc1ccccc1C(C)(C)C
<b>Mol. weight [g/mol]:</b>	163.26
<b>CAS:</b>	109932-97-0

## Physical Properties

Property code	Value	Unit	Source
gf	236.75	kJ/mol	Joback Method
hf	-0.59	kJ/mol	Joback Method
hfus	15.58	kJ/mol	Joback Method
hvap	48.16	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	3.026		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
tb	529.68	K	Joback Method
tc	747.19	K	Joback Method
tf	307.75	K	Joback Method
vc	0.568	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.99	J/molxK	529.68	Joback Method
cpg	370.79	J/molxK	565.93	Joback Method
cpg	386.49	J/molxK	602.18	Joback Method
cpg	401.16	J/molxK	638.44	Joback Method
cpg	414.86	J/molxK	674.69	Joback Method
cpg	427.64	J/molxK	710.94	Joback Method
cpg	439.56	J/molxK	747.19	Joback Method

# Sources

<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=C109932970&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C109932970&amp;Units=SI</a>
<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>

# 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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