

# Aniline, 4-tert-amyl-2-methyl-

<b>Inchi:</b>	InChI=1S/C12H19N/c1-5-12(3,4)10-6-7-11(13)9(2)8-10/h6-8H,5,13H2,1-4H3
<b>InchiKey:</b>	YPSTYABUNGSLQO-UHFFFAOYSA-N
<b>Formula:</b>	C12H19N
<b>SMILES:</b>	CCC(C)(C)c1ccc(N)c(C)c1
<b>Mol. weight [g/mol]:</b>	177.29

## Physical Properties

Property code	Value	Unit	Source
gf	212.60	kJ/mol	Joback Method
hf	-52.38	kJ/mol	Joback Method
hfus	17.88	kJ/mol	Joback Method
hvap	55.25	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.265		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
tb	579.90	K	Joback Method
tc	803.73	K	Joback Method
tf	362.14	K	Joback Method
vc	0.618	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.91	J/molxK	579.90	Joback Method
cpg	430.72	J/molxK	617.21	Joback Method
cpg	446.46	J/molxK	654.51	Joback Method
cpg	461.16	J/molxK	691.82	Joback Method
cpg	474.91	J/molxK	729.12	Joback Method
cpg	487.74	J/molxK	766.43	Joback Method
cpg	499.74	J/molxK	803.73	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=B6008475&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008475&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>

# 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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