

# Aniline, 2,4-dimethyl-6-tert-butyl-

<b>Inchi:</b>	InChI=1S/C12H19N/c1-8-6-9(2)11(13)10(7-8)12(3,4)5/h6-7H,13H2,1-5H3
<b>InchiKey:</b>	SJMVAOMOFSHXEH-UHFFFAOYSA-N
<b>Formula:</b>	C12H19N
<b>SMILES:</b>	<chem>Cc1cc(C)c(N)c(C(C)(C)C)c1</chem>
<b>Mol. weight [g/mol]:</b>	177.29
<b>CAS:</b>	35735-32-1

## Physical Properties

Property code	Value	Unit	Source
gf	202.97	kJ/mol	Joback Method
hf	-63.85	kJ/mol	Joback Method
hfus	17.49	kJ/mol	Joback Method
hvap	55.91	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.183		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
tb	584.88	K	Joback Method
tc	809.73	K	Joback Method
tf	374.66	K	Joback Method
vc	0.618	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.68	J/molxK	584.88	Joback Method
cpg	430.20	J/molxK	622.36	Joback Method
cpg	445.70	J/molxK	659.83	Joback Method
cpg	460.22	J/molxK	697.31	Joback Method
cpg	473.82	J/molxK	734.78	Joback Method
cpg	486.55	J/molxK	772.26	Joback Method
cpg	498.46	J/molxK	809.73	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=C35735321&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C35735321&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>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

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