

# Acetamide, N-[4-(1,1-dimethylethyl)phenyl]-

<b>Other names:</b>	Acetanilide, 4'-tert-butyl- 4'-tert-Butylacetanilide p-tert-Butylacetanilide
<b>Inchi:</b>	InChI=1S/C12H17NO/c1-9(14)13-11-7-5-10(6-8-11)12(2,3)4/h5-8H,1-4H3,(H,13,14)
<b>InchiKey:</b>	RMUYDDKCUZHVHY-UHFFFAOYSA-N
<b>Formula:</b>	C12H17NO
<b>SMILES:</b>	CC(=O)Nc1ccc(C(C)(C)C)cc1
<b>Mol. weight [g/mol]:</b>	191.27
<b>CAS:</b>	20330-45-4

## Physical Properties

Property code	Value	Unit	Source
gf	116.25	kJ/mol	Joback Method
hf	-133.81	kJ/mol	Joback Method
hfus	19.77	kJ/mol	Joback Method
hvap	57.13	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.942		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
tb	606.43	K	Joback Method
tc	827.99	K	Joback Method
tf	368.95	K	Joback Method
vc	0.629	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.85	J/molxK	606.43	Joback Method
cpg	438.62	J/molxK	643.36	Joback Method
cpg	453.30	J/molxK	680.28	Joback Method
cpg	466.95	J/molxK	717.21	Joback Method
cpg	479.65	J/molxK	754.13	Joback Method
cpg	491.44	J/molxK	791.06	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C20330454&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20330454&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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