

# tert-butyl-n-amyl-amine

<b>Inchi:</b>	InChI=1S/C9H21N/c1-5-6-7-8-10-9(2,3)4/h10H,5-8H2,1-4H3
<b>InchiKey:</b>	PKKKSUKYKSPFSS-UHFFFAOYSA-N
<b>Formula:</b>	C9H21N
<b>SMILES:</b>	CCCCCNC(C)(C)C
<b>Mol. weight [g/mol]:</b>	143.27

## Physical Properties

Property code	Value	Unit	Source
gf	117.13	kJ/mol	Joback Method
hf	-184.37	kJ/mol	Joback Method
hfus	16.75	kJ/mol	Joback Method
hvap	40.77	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.565		Crippen Method
mcvol	147.650	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
rinpola	937.00		NIST Webbook
tb	452.26	K	Joback Method
tc	629.87	K	Joback Method
tf	246.27	K	Joback Method
vc	0.564	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.96	J/mol×K	452.26	Joback Method
cpg	340.84	J/mol×K	481.86	Joback Method
cpg	355.97	J/mol×K	511.46	Joback Method
cpg	370.39	J/mol×K	541.06	Joback Method
cpg	384.10	J/mol×K	570.67	Joback Method
cpg	397.15	J/mol×K	600.27	Joback Method
cpg	409.56	J/mol×K	629.87	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R521870&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R521870&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>
<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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<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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