

# N-butyl-p-toluidine

<b>Inchi:</b>	InChI=1S/C11H17N/c1-3-4-9-12-11-7-5-10(2)6-8-11/h5-8,12H,3-4,9H2,1-2H3
<b>InchiKey:</b>	FPHFMZTUFVNDQL-UHFFFAOYSA-N
<b>Formula:</b>	C11H17N
<b>SMILES:</b>	CCCCNc1ccc(C)cc1
<b>Mol. weight [g/mol]:</b>	163.26
<b>CAS:</b>	10387-24-3

## Physical Properties

Property code	Value	Unit	Source
gf	233.91	kJ/mol	Joback Method
hf	8.16	kJ/mol	Joback Method
hfus	23.00	kJ/mol	Joback Method
hvap	49.45	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.207		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
tb	532.91	K	Joback Method
tc	737.35	K	Joback Method
tf	305.33	K	Joback Method
vc	0.579	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.85	J/molxK	532.91	Joback Method
cpg	366.50	J/molxK	566.98	Joback Method
cpg	381.31	J/molxK	601.06	Joback Method
cpg	395.29	J/molxK	635.13	Joback Method
cpg	408.50	J/molxK	669.20	Joback Method
cpg	420.94	J/molxK	703.27	Joback Method
cpg	432.67	J/molxK	737.35	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=C10387243&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10387243&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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