

# 2-(N-Ethyl-N-toluidino)ethanol, acetate

<b>Inchi:</b>	InChI=1S/C13H19NO2/c1-4-14(8-9-16-12(3)15)13-7-5-6-11(2)10-13/h5-7,10H,4,8-9H2,1
<b>InchiKey:</b>	KMLMCHZWMDCYPI-UHFFFAOYSA-N
<b>Formula:</b>	C13H19NO2
<b>SMILES:</b>	CCN(CCOC(C)=O)c1cccc(C)c1
<b>Mol. weight [g/mol]:</b>	221.30

## Physical Properties

Property code	Value	Unit	Source
gf	38.22	kJ/mol	Joback Method
hf	-263.86	kJ/mol	Joback Method
hfus	28.89	kJ/mol	Joback Method
hvap	58.67	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.384		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1671.40		NIST Webbook
rinpol	1671.40		NIST Webbook
tb	617.23	K	Joback Method
tc	818.49	K	Joback Method
tf	379.84	K	Joback Method
vc	0.698	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.53	J/molxK	617.23	Joback Method
cpg	496.49	J/molxK	650.77	Joback Method
cpg	511.54	J/molxK	684.32	Joback Method
cpg	525.72	J/molxK	717.86	Joback Method
cpg	539.05	J/molxK	751.40	Joback Method
cpg	551.56	J/molxK	784.95	Joback Method
cpg	563.27	J/molxK	818.49	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=U352275&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U352275&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</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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