

# N-Acetylnortriptyline

<b>Other names:</b>	Noramitriptyline acetylated
<b>Inchi:</b>	InChI=1S/C21H23NO/c1-16(23)22(2)15-7-12-21-19-10-5-3-8-17(19)13-14-18-9-4-6-11-2
<b>InchiKey:</b>	CDGDSKQTZFJQQF-UHFFFAOYSA-N
<b>Formula:</b>	C21H23NO
<b>SMILES:</b>	CC(=O)N(C)CCC=C1c2ccccc2CCc2ccccc21
<b>Mol. weight [g/mol]:</b>	305.41
<b>CAS:</b>	16234-90-5

## Physical Properties

Property code	Value	Unit	Source
gf	427.28	kJ/mol	Joback Method
hf	97.47	kJ/mol	Joback Method
hfus	39.46	kJ/mol	Joback Method
hvap	78.01	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.085		Crippen Method
mcvol	255.620	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	2660.00		NIST Webbook
rinpol	2660.00		NIST Webbook
tb	827.56	K	Joback Method
tc	1060.84	K	Joback Method
tf	519.25	K	Joback Method
vc	0.961	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.64	J/molxK	827.56	Joback Method
cpg	776.19	J/molxK	866.44	Joback Method
cpg	791.67	J/molxK	905.32	Joback Method
cpg	806.22	J/molxK	944.20	Joback Method
cpg	819.98	J/molxK	983.08	Joback Method
cpg	833.09	J/molxK	1021.96	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C16234905&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16234905&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>

## 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>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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