

# Toliprolol - H2O, acetylated

<b>Inchi:</b>	InChI=1S/C15H21NO2/c1-12(2)16(14(4)17)9-6-10-18-15-8-5-7-13(3)11-15/h5-9,11-12H,
<b>InchiKey:</b>	NARJAWFSQHVZJD-RMKNXTFCSA-N
<b>Formula:</b>	C15H21NO2
<b>SMILES:</b>	CC(=O)N(C=CCOc1cccc(C)c1)C(C)C
<b>Mol. weight [g/mol]:</b>	247.33

## Physical Properties

Property code	Value	Unit	Source
gf	132.84	kJ/mol	Joback Method
hf	-193.20	kJ/mol	Joback Method
hfus	30.75	kJ/mol	Joback Method
hvap	62.69	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.144		Crippen Method
mcvol	211.570	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinqol	2230.00		NIST Webbook
tb	666.71	K	Joback Method
tc	873.77	K	Joback Method
tf	382.30	K	Joback Method
vc	0.783	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.94	J/molxK	666.71	Joback Method
cpg	580.62	J/molxK	701.22	Joback Method
cpg	596.27	J/molxK	735.73	Joback Method
cpg	610.94	J/molxK	770.24	Joback Method
cpg	624.69	J/molxK	804.75	Joback Method
cpg	637.54	J/molxK	839.26	Joback Method
cpg	649.56	J/molxK	873.77	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R583096&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R583096&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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