

# Toliprolol desamino hydroxy, acetylated

<b>Inchi:</b>	InChI=1S/C14H18O5/c1-10-5-4-6-13(7-10)18-9-14(19-12(3)16)8-17-11(2)15/h4-7,14H,8
<b>InchiKey:</b>	YBZAUDYBEYBZHG-UHFFFAOYSA-N
<b>Formula:</b>	C14H18O5
<b>SMILES:</b>	CC(=O)OCC(COc1cccc(C)c1)OC(C)=O
<b>Mol. weight [g/mol]:</b>	266.29

## Physical Properties

Property code	Value	Unit	Source
gf	-405.50	kJ/mol	Joback Method
hf	-734.33	kJ/mol	Joback Method
hfus	28.91	kJ/mol	Joback Method
hvap	70.03	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	1.869		Crippen Method
mcvol	205.110	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook
tb	725.94	K	Joback Method
tc	933.66	K	Joback Method
tf	438.03	K	Joback Method
vc	0.771	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.18	J/molxK	725.94	Joback Method
cpg	629.17	J/molxK	899.04	Joback Method
cpg	618.70	J/molxK	864.42	Joback Method
cpg	607.26	J/molxK	829.80	Joback Method
cpg	594.85	J/molxK	795.18	Joback Method
cpg	581.49	J/molxK	760.56	Joback Method
cpg	638.67	J/molxK	933.66	Joback Method
dvisc	0.0000849	Paxs	725.94	Joback Method

dvisc	0.0001085	Paxs	677.96	Joback Method
dvisc	0.0001438	Paxs	629.97	Joback Method
dvisc	0.0001996	Paxs	581.99	Joback Method
dvisc	0.0002940	Paxs	534.00	Joback Method
dvisc	0.0004673	Paxs	486.02	Joback Method
dvisc	0.0008224	Paxs	438.03	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R583081&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R583081&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>dvisc:</b>	Dynamic viscosity
<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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