

# Alprenolol, N,O-di(acetyl)-

<b>Other names:</b>	Alprenolol, acetylated
<b>Inchi:</b>	InChI=1S/C19H27NO4/c1-6-9-17-10-7-8-11-19(17)23-13-18(24-16(5)22)12-20(14(2)3)15
<b>InchiKey:</b>	JULCEMKDOVJFID-UHFFFAOYSA-N
<b>Formula:</b>	C19H27NO4
<b>SMILES:</b>	<chem>C=CCc1cccc1OCC(CN(C(C)=O)C(C)C)OC(C)=O</chem>
<b>Mol. weight [g/mol]:</b>	333.42
<b>CAS:</b>	959081-88-0

## Physical Properties

Property code	Value	Unit	Source
gf	-62.22	kJ/mol	Joback Method
hf	-517.63	kJ/mol	Joback Method
hfus	38.89	kJ/mol	Joback Method
hvap	79.73	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	2.982		Crippen Method
mcvol	275.370	ml/mol	McGowan Method
pc	1504.65	kPa	Joback Method
rinpol	2275.00		NIST Webbook
rinpol	2275.00		NIST Webbook
tb	826.60	K	Joback Method
tc	1031.57	K	Joback Method
tf	487.86	K	Joback Method
vc	1.026	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.16	J/molxK	826.60	Joback Method
cpg	850.91	J/molxK	860.76	Joback Method
cpg	865.52	J/molxK	894.92	Joback Method
cpg	879.01	J/molxK	929.08	Joback Method
cpg	891.43	J/molxK	963.24	Joback Method
cpg	902.80	J/molxK	997.40	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=C959081880&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C959081880&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>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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