

# Levobunolol - H2O, acetylated

**Inchi:** InChI=1S/C20H27NO2/c1-15(22)21(20(2,3)4)14-6-5-9-16-10-7-12-18-17(16)11-8-13-19(  
**InchiKey:** ACEZFNAHCYRECY-NSIKDUERSA-N  
**Formula:** C20H27NO2  
**SMILES:** CC(=O)N(C=CCCc1cccc2c1CCCC2=O)C(C)(C)C  
**Mol. weight [g/mol]:** 313.43

## Physical Properties

Property code	Value	Unit	Source
gf	209.36	kJ/mol	Joback Method
hf	-229.84	kJ/mol	Joback Method
hfus	32.70	kJ/mol	Joback Method
hvap	75.81	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.299		Crippen Method
mcvol	266.860	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinsol	2570.00		NIST Webbook
tb	844.38	K	Joback Method
tc	1074.03	K	Joback Method
tf	533.24	K	Joback Method
vc	0.998	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.20	J/molxK	844.38	Joback Method
cpg	851.73	J/molxK	882.65	Joback Method
cpg	868.05	J/molxK	920.93	Joback Method
cpg	883.29	J/molxK	959.20	Joback Method
cpg	897.55	J/molxK	997.48	Joback Method
cpg	910.95	J/molxK	1035.75	Joback Method
cpg	923.61	J/molxK	1074.03	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=R582677&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R582677&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>

# 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>hvac:</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>mccol:</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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