

# Bunitrolol hydroxy, acetylated

<b>Inchi:</b>	InChI=1S/C20H26N2O6/c1-13(23)22(20(4,5)6)11-18(28-15(3)25)12-26-19-8-7-17(27-14)
<b>InchiKey:</b>	QEODEMLNRPFUAD-UHFFFAOYSA-N
<b>Formula:</b>	C20H26N2O6
<b>SMILES:</b>	CC(=O)Oc1ccc(OCC(CN(C(C)=O)C(C)(C)C)OC(C)=O)c(C#N)c1
<b>Mol. weight [g/mol]:</b>	390.43

## Physical Properties

Property code	Value	Unit	Source
gf	-246.73	kJ/mol	Joback Method
hf	-758.56	kJ/mol	Joback Method
hfus	42.77	kJ/mol	Joback Method
hvap	102.02	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	2.441		Crippen Method
mcvol	302.580	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
tb	1033.36	K	Joback Method
tc	1267.43	K	Joback Method
tf	667.98	K	Joback Method
vc	1.147	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	975.27	J/molxK	1033.36	Joback Method
cpg	985.22	J/molxK	1072.37	Joback Method
cpg	993.75	J/molxK	1111.38	Joback Method
cpg	1000.92	J/molxK	1150.40	Joback Method
cpg	1006.75	J/molxK	1189.41	Joback Method
cpg	1011.29	J/molxK	1228.42	Joback Method
cpg	1014.59	J/molxK	1267.43	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R582533&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R582533&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>hvp:</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>rinp:</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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