

# 2-Acetoxy-1-(N-acetyl-N-isopropyl)amino-3-(4-ace

<b>Other names:</b>	Alprenolol, hydroxy, acetylated
<b>Inchi:</b>	InChI=1S/C21H29NO6/c1-7-8-18-11-19(27-16(5)24)9-10-21(18)26-13-20(28-17(6)25)12
<b>InchiKey:</b>	LBOSTHQFSRFOGE-UHFFFAOYSA-N
<b>Formula:</b>	C21H29NO6
<b>SMILES:</b>	<chem>C=CCc1cc(OC(C)=O)ccc1OCC(CN(C(C)=O)C(C)C)OC(C)=O</chem>
<b>Mol. weight [g/mol]:</b>	391.46

## Physical Properties

Property code	Value	Unit	Source
gf	-288.93	kJ/mol	Joback Method
hf	-815.18	kJ/mol	Joback Method
hfus	46.46	kJ/mol	Joback Method
hvap	94.01	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	2.908		Crippen Method
mvol	310.990	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	2575.00		NIST Webbook
tb	953.63	K	Joback Method
tc	1171.02	K	Joback Method
tf	595.08	K	Joback Method
vc	1.163	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	994.53	J/molxK	953.63	Joback Method
cpg	1007.82	J/molxK	989.86	Joback Method
cpg	1019.69	J/molxK	1026.09	Joback Method
cpg	1030.16	J/molxK	1062.33	Joback Method
cpg	1039.25	J/molxK	1098.56	Joback Method
cpg	1046.99	J/molxK	1134.79	Joback Method
cpg	1053.40	J/molxK	1171.02	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=U281340&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U281340&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</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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