

# 1,2-Diacetoxy-3-[4-acetoxy-2-(2-acetoxy)propyl]ph

<b>Other names:</b>	Alprenolol desaminodihydroxy + H <sub>2</sub> O, acetylated
<b>Inchi:</b>	InChI=1S/C20H26O9/c1-12(27-14(3)22)8-17-9-18(28-15(4)23)6-7-20(17)26-11-19(29-16
<b>InchiKey:</b>	XCGBFJXUDBUTAP-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>20</sub> H <sub>26</sub> O <sub>9</sub>
<b>SMILES:</b>	CC(=O)OCC(COc1ccc(OC(C)=O)cc1CC(C)OC(C)=O)OC(C)=O
<b>Mol. weight [g/mol]:</b>	410.42

## Physical Properties

Property code	Value	Unit	Source
gf	-834.89	kJ/mol	Joback Method
hf	-1364.52	kJ/mol	Joback Method
hfus	46.11	kJ/mol	Joback Method
hvap	101.97	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	1.980		Crippen Method
mvol	304.530	ml/mol	McGowan Method
pc	1419.71	kPa	Joback Method
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook
tb	1020.34	K	Joback Method
tc	1249.73	K	Joback Method
tf	647.49	K	Joback Method
vc	1.149	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	981.77	J/molxK	1020.34	Joback Method
cpg	1006.37	J/molxK	1211.50	Joback Method
cpg	1005.59	J/molxK	1173.27	Joback Method
cpg	1002.71	J/molxK	1135.04	Joback Method
cpg	997.75	J/molxK	1096.80	Joback Method
cpg	990.76	J/molxK	1058.57	Joback Method
cpg	1005.01	J/molxK	1249.73	Joback Method

dvisc	0.0000170	Paxs	1020.34	Joback Method
dvisc	0.0000216	Paxs	958.20	Joback Method
dvisc	0.0000285	Paxs	896.06	Joback Method
dvisc	0.0000390	Paxs	833.91	Joback Method
dvisc	0.0000563	Paxs	771.77	Joback Method
dvisc	0.0000866	Paxs	709.63	Joback Method
dvisc	0.0001447	Paxs	647.49	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=U281341&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U281341&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>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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