

# 31-Norcyclolaudenol acetate

<b>Inchi:</b>	InChI=1S/C32H52O2/c1-20(2)21(3)9-10-22(4)24-11-12-25-26-13-14-27-29(6,7)28(34-23
<b>InchiKey:</b>	QIUMNCOQNZKHEF-MNTLUMBWSA-N
<b>Formula:</b>	C32H52O2
<b>SMILES:</b>	C=C(C)C(C)CCC(C)C1CCC2C3CCC4C(C)(C)C(OC(C)=O)CCC45CC35CCC12C
<b>Mol. weight [g/mol]:</b>	468.75

## Physical Properties

Property code	Value	Unit	Source
gf	273.70	kJ/mol	Joback Method
hf	-518.41	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	88.86	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.596		Crippen Method
mvol	410.580	ml/mol	McGowan Method
pc	861.00	kPa	Joback Method
rinpol	3367.00		NIST Webbook
rinpol	3367.00		NIST Webbook
tb	1032.32	K	Joback Method
tc	1270.96	K	Joback Method
tf	634.62	K	Joback Method
vc	1.571	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1649.30	J/molxK	1032.32	Joback Method
cpg	1700.86	J/molxK	1072.09	Joback Method
cpg	1756.63	J/molxK	1111.87	Joback Method
cpg	1817.30	J/molxK	1151.64	Joback Method
cpg	1883.55	J/molxK	1191.41	Joback Method
cpg	1956.06	J/molxK	1231.19	Joback Method
cpg	2035.52	J/molxK	1270.96	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=R110673&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R110673&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>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>rlnpol:</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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