

# 7-Tirucallenol acetate

**Inchi:** InChI=1S/C32H54O2/c1-21(2)11-10-12-22(3)24-15-19-32(9)26-13-14-27-29(5,6)28(34-2  
**InchiKey:** KKIPVJGDVKRFSF-JNYOTSAWSA-N  
**Formula:** C32H54O2  
**SMILES:** CC(=O)OC1CCC2(C)C3CCC4(C)C(C(C)CCCC(C)C)CCC4(C)C3=CCC2C1(C)C  
**Mol. weight [g/mol]:** 470.77

## Physical Properties

Property code	Value	Unit	Source
gf	129.79	kJ/mol	Joback Method
hf	-672.86	kJ/mol	Joback Method
hfus	36.34	kJ/mol	Joback Method
hvap	90.83	kJ/mol	Joback Method
log10ws	-9.45		Crippen Method
logp	8.986		Crippen Method
mvol	421.440	ml/mol	McGowan Method
pc	809.83	kPa	Joback Method
rinpol	3358.00		NIST Webbook
rinpol	3358.00		NIST Webbook
tb	1041.70	K	Joback Method
tc	1279.77	K	Joback Method
tf	638.64	K	Joback Method
vc	1.601	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1677.94	J/molxK	1041.70	Joback Method
cpg	1728.28	J/molxK	1081.38	Joback Method
cpg	1782.26	J/molxK	1121.06	Joback Method
cpg	1840.47	J/molxK	1160.73	Joback Method
cpg	1903.53	J/molxK	1200.41	Joback Method
cpg	1972.04	J/molxK	1240.09	Joback Method
cpg	2046.59	J/molxK	1279.77	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=R110935&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R110935&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>
<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>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>rinpola:</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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