

# Kolavenol acetate

<b>Inchi:</b>	InChI=1S/C22H36O2/c1-16(12-15-24-19(4)23)10-13-21(5)18(3)11-14-22(6)17(2)8-7-9-20
<b>InchiKey:</b>	XAYGDGVRGSNBDV-FOWTUZBSSA-N
<b>Formula:</b>	C22H36O2
<b>SMILES:</b>	CC(=O)OCC=C(C)CCC1(C)C(C)CCC2(C)C(C)=CCCC21
<b>Mol. weight [g/mol]:</b>	332.52
<b>CAS:</b>	19941-84-5

## Physical Properties

Property code	Value	Unit	Source
gf	39.14	kJ/mol	Joback Method
hf	-477.71	kJ/mol	Joback Method
hfus	32.66	kJ/mol	Joback Method
hvap	72.31	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	6.075		Crippen Method
mcvol	297.960	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
rinpol	2411.90		NIST Webbook
rinpol	2411.90		NIST Webbook
tb	808.93	K	Joback Method
tc	1025.15	K	Joback Method
tf	465.22	K	Joback Method
vc	1.135	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.34	J/molxK	808.93	Joback Method
cpg	987.72	J/molxK	844.97	Joback Method
cpg	1011.72	J/molxK	881.00	Joback Method
cpg	1035.57	J/molxK	917.04	Joback Method
cpg	1059.52	J/molxK	953.08	Joback Method
cpg	1083.79	J/molxK	989.11	Joback Method
cpg	1108.62	J/molxK	1025.15	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C19941845&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19941845&amp;Units=SI</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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