

# 5,25-Ergostadienol acetate

<b>Inchi:</b>	InChI=1S/C30H48O2/c1-19(2)20(3)8-9-21(4)26-12-13-27-25-11-10-23-18-24(32-22(5)31
<b>InchiKey:</b>	LGWPVSYEGQFZII-GLBIWXSHSA-N
<b>Formula:</b>	C30H48O2
<b>SMILES:</b>	<chem>C=C(C)C(C)CCC(C)C1CCC2C3CC=C4CC(OC(C)=O)CCC4(C)C3CCC12C</chem>
<b>Mol. weight [g/mol]:</b>	440.70

## Physical Properties

Property code	Value	Unit	Source
gf	210.93	kJ/mol	Joback Method
hf	-526.08	kJ/mol	Joback Method
hfus	40.10	kJ/mol	Joback Method
hvap	88.40	kJ/mol	Joback Method
log10ws	-8.71		Crippen Method
logp	8.126		Crippen Method
mvol	388.960	ml/mol	McGowan Method
pc	900.72	kPa	Joback Method
rinpol	3260.00		NIST Webbook
tb	996.69	K	Joback Method
tc	1229.29	K	Joback Method
tf	556.82	K	Joback Method
vc	1.476	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1472.17	J/molxK	996.69	Joback Method
cpg	1505.66	J/molxK	1035.46	Joback Method
cpg	1539.89	J/molxK	1074.22	Joback Method
cpg	1575.24	J/molxK	1112.99	Joback Method
cpg	1612.05	J/molxK	1151.76	Joback Method
cpg	1650.70	J/molxK	1190.52	Joback Method
cpg	1691.54	J/molxK	1229.29	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=R110806&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R110806&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>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>mccvol:</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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