

# 7,22,25-Stigmastatrienol acetate, 24-«beta»

<b>Inchi:</b>	InChI=1S/C31H48O2/c1-8-23(20(2)3)10-9-21(4)27-13-14-28-26-12-11-24-19-25(33-22(5
<b>InchiKey:</b>	YOXXESRXSQRNHU-NYDNHBLDSA-N
<b>Formula:</b>	C31H48O2
<b>SMILES:</b>	<chem>C=C(C)C(C=CC(C)C1CCC2C3=CCC4CC(OC(C)=O)CCC4(C)C3CCC21C)CC</chem>
<b>Mol. weight [g/mol]:</b>	452.71

## Physical Properties

Property code	Value	Unit	Source
gf	299.57	kJ/mol	Joback Method
hf	-429.50	kJ/mol	Joback Method
hfus	42.89	kJ/mol	Joback Method
hvap	90.58	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	8.292		Crippen Method
mcvol	398.750	ml/mol	McGowan Method
pc	877.39	kPa	Joback Method
rinsol	3350.00		NIST Webbook
tb	1023.73	K	Joback Method
tc	1261.05	K	Joback Method
tf	563.01	K	Joback Method
vc	1.512	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1516.89	J/mol×K	1023.73	Joback Method
cpg	1552.36	J/mol×K	1063.28	Joback Method
cpg	1589.04	J/mol×K	1102.84	Joback Method
cpg	1627.34	J/mol×K	1142.39	Joback Method
cpg	1667.65	J/mol×K	1181.94	Joback Method
cpg	1710.39	J/mol×K	1221.50	Joback Method
cpg	1755.98	J/mol×K	1261.05	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=R110851&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R110851&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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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