

# Peposterol (7,24-Stigmastadienol) acetate

<b>Inchi:</b>	InChI=1S/C31H50O2/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>	JFVZFDYSNAYWDL-FETVILCLSA-N
<b>Formula:</b>	C31H50O2
<b>SMILES:</b>	CCC(CCC(C)C1CCC2C3=CCC4CC(OC(C)=O)CCC4(C)C3CCC21C)=C(C)C
<b>Mol. weight [g/mol]:</b>	454.73

## Physical Properties

Property code	Value	Unit	Source
gf	205.62	kJ/mol	Joback Method
hf	-559.44	kJ/mol	Joback Method
hfus	46.38	kJ/mol	Joback Method
hvap	91.72	kJ/mol	Joback Method
log10ws	-9.37		Crippen Method
logp	8.660		Crippen Method
mcvol	403.050	ml/mol	McGowan Method
pc	854.46	kPa	Joback Method
rinsol	3443.00		NIST Webbook
tb	1027.37	K	Joback Method
tc	1263.47	K	Joback Method
tf	565.81	K	Joback Method
vc	1.538	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1548.25	J/molxK	1027.37	Joback Method
cpg	1584.19	J/molxK	1066.72	Joback Method
cpg	1621.28	J/molxK	1106.07	Joback Method
cpg	1659.92	J/molxK	1145.42	Joback Method
cpg	1700.51	J/molxK	1184.77	Joback Method
cpg	1743.43	J/molxK	1224.12	Joback Method
cpg	1789.10	J/molxK	1263.47	Joback Method

# Sources

<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=R111394&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R111394&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvac:</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>mccol:</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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