

# 22-Stigmastenol acetate

<b>Inchi:</b>	InChI=1S/C31H52O2/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>	MAIIZFGSYSUIIV-RBQRRVTJSA-N
<b>Formula:</b>	C31H52O2
<b>SMILES:</b>	CCC(CCC(C)C1CCC2C3=CCC4CC(OC(C)=O)CCC4(C)C3CCC21C)C(C)C
<b>Mol. weight [g/mol]:</b>	456.74

## Physical Properties

Property code	Value	Unit	Source
gf	137.62	kJ/mol	Joback Method
hf	-667.64	kJ/mol	Joback Method
hfus	41.75	kJ/mol	Joback Method
hvap	90.83	kJ/mol	Joback Method
log10ws	-9.03		Crippen Method
logp	8.596		Crippen Method
mvol	407.350	ml/mol	McGowan Method
pc	831.94	kPa	Joback Method
rinpol	3318.00		NIST Webbook
rinpol	3318.00		NIST Webbook
tb	1022.57	K	Joback Method
tc	1255.94	K	Joback Method
tf	568.81	K	Joback Method
vc	1.544	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1576.09	J/molxK	1022.57	Joback Method
cpg	1611.24	J/molxK	1061.47	Joback Method
cpg	1647.21	J/molxK	1100.36	Joback Method
cpg	1684.37	J/molxK	1139.26	Joback Method
cpg	1723.09	J/molxK	1178.15	Joback Method
cpg	1763.71	J/molxK	1217.05	Joback Method
cpg	1806.62	J/molxK	1255.94	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=R489855&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R489855&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>

# 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>hvp:</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>rinp:</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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