

# 4A-Methyl-8(14)-stigmastenol acetate

<b>Inchi:</b>	InChI=1S/C32H54O2/c1-9-24(20(2)3)11-10-21(4)26-14-15-28-25-12-13-27-22(5)30(34-2
<b>InchiKey:</b>	XVXYPWSUIYJWOZ-QMTMGZM RSA-N
<b>Formula:</b>	C32H54O2
<b>SMILES:</b>	CCC(CCC(C)C1CCC2=C3CCC4C(C)C(OC(C)=O)CCC4(C)C3CCC21C)C(C)C
<b>Mol. weight [g/mol]:</b>	470.77

## Physical Properties

Property code	Value	Unit	Source
gf	136.41	kJ/mol	Joback Method
hf	-699.75	kJ/mol	Joback Method
hfus	43.95	kJ/mol	Joback Method
hvap	93.72	kJ/mol	Joback Method
log10ws	-9.45		Crippen Method
logp	8.986		Crippen Method
mcvol	421.440	ml/mol	McGowan Method
pc	781.12	kPa	Joback Method
rinsol	3408.00		NIST Webbook
tb	1050.43	K	Joback Method
tc	1287.54	K	Joback Method
tf	592.60	K	Joback Method
vc	1.601	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1650.78	J/mol×K	1050.43	Joback Method
cpg	1687.77	J/mol×K	1089.95	Joback Method
cpg	1725.79	J/mol×K	1129.47	Joback Method
cpg	1765.22	J/mol×K	1168.98	Joback Method
cpg	1806.43	J/mol×K	1208.50	Joback Method
cpg	1849.81	J/mol×K	1248.02	Joback Method
cpg	1895.72	J/mol×K	1287.54	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=R110722&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R110722&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>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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