

# 5«alpha»-Stigmastan-3«beta»-ol

<b>Other names:</b>	(3«beta»,5«alpha»)-stigmastan-3-ol Stigmastanol
<b>Inchi:</b>	InChI=1S/C29H52O/c1-7-21(19(2)3)9-8-20(4)25-12-13-26-24-11-10-22-18-23(30)14-16-2
<b>InchiKey:</b>	LGJMUZUPVCAVPU-LRTHRWAWSA-N
<b>Formula:</b>	C29H52O
<b>SMILES:</b>	CCC(CCC(C)C1CCC2C3CCC4CC(O)CCC4(C)C3CCC12C)C(C)C
<b>Mol. weight [g/mol]:</b>	416.72
<b>CAS:</b>	83-45-4

## Physical Properties

Property code	Value	Unit	Source
gf	189.84	kJ/mol	Joback Method
hf	-600.44	kJ/mol	Joback Method
hfus	38.11	kJ/mol	Joback Method
hvap	92.64	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	8.105		Crippen Method
mcvol	381.900	ml/mol	McGowan Method
pc	927.81	kPa	Joback Method
rinpol	3260.00		NIST Webbook
rinpol	3325.00		NIST Webbook
rinpol	3290.00		NIST Webbook
rinpol	3317.00		NIST Webbook
tb	983.89	K	Joback Method
tc	1207.73	K	Joback Method
tf	517.41	K	Joback Method
vc	1.440	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1490.57	J/mol×K	983.89	Joback Method
cpg	1523.85	J/mol×K	1021.20	Joback Method
cpg	1557.68	J/mol×K	1058.50	Joback Method

cpg	1592.42	J/mol×K	1095.81	Joback Method
cpg	1628.38	J/mol×K	1133.11	Joback Method
cpg	1665.90	J/mol×K	1170.42	Joback Method
cpg	1705.32	J/mol×K	1207.73	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C83454&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C83454&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>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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