

# 5«alpha»-Stigmast-7-en-3-one

<b>Inchi:</b>	InChI=1S/C29H48O/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>	JWANJDUXWSJWER-WHNXKXCLSA-N
<b>Formula:</b>	C29H48O
<b>SMILES:</b>	CCC(CCC(C)C1CCC2C3=CCC4CC(=O)CCC4(C)C3CCC21C)C(C)C
<b>Mol. weight [g/mol]:</b>	412.69

## Physical Properties

Property code	Value	Unit	Source
gf	239.82	kJ/mol	Joback Method
hf	-498.92	kJ/mol	Joback Method
hfus	32.23	kJ/mol	Joback Method
hvap	81.78	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	8.233		Crippen Method
mvol	373.300	ml/mol	McGowan Method
pc	945.00	kPa	Joback Method
rinpol	3420.00		NIST Webbook
rinpol	3420.00		NIST Webbook
tb	973.01	K	Joback Method
tc	1207.19	K	Joback Method
tf	546.57	K	Joback Method
vc	1.417	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1414.77	J/mol×K	973.01	Joback Method
cpg	1447.96	J/mol×K	1012.04	Joback Method
cpg	1481.61	J/mol×K	1051.07	Joback Method
cpg	1516.07	J/mol×K	1090.10	Joback Method
cpg	1551.70	J/mol×K	1129.13	Joback Method
cpg	1588.83	J/mol×K	1168.16	Joback Method
cpg	1627.84	J/mol×K	1207.19	Joback Method

# Sources

<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=R641093&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R641093&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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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