

5«alpha»-Stigmast-8(14)-en-3-one

Inchi:	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
InchiKey:	PMEZZMJCMAZPKD-UHSXNZBRSA-N
Formula:	C29H48O
SMILES:	CCC(CCC(C)C1CCC2=C3CCC4CC(=O)CCC4(C)C3CCC21C)C(C)C
Mol. weight [g/mol]:	412.69

Physical Properties

Property code	Value	Unit	Source
gf	237.90	kJ/mol	Joback Method
hf	-490.05	kJ/mol	Joback Method
hfus	30.77	kJ/mol	Joback Method
hvap	82.75	kJ/mol	Joback Method
log10ws	-8.74		Crippen Method
logp	8.377		Crippen Method
mcvol	373.300	ml/mol	McGowan Method
pc	955.55	kPa	Joback Method
rinpol	3285.00		NIST Webbook
tb	982.66	K	Joback Method
tc	1217.96	K	Joback Method
tf	563.33	K	Joback Method
vc	1.417	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1413.26	J/mol×K	982.66	Joback Method
cpg	1446.70	J/mol×K	1021.88	Joback Method
cpg	1480.76	J/mol×K	1061.09	Joback Method
cpg	1515.80	J/mol×K	1100.31	Joback Method
cpg	1552.18	J/mol×K	1139.53	Joback Method
cpg	1590.25	J/mol×K	1178.75	Joback Method
cpg	1630.37	J/mol×K	1217.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R528777&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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