

Stigmasta-5,23-dien-3«beta»-ol

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:	JNYKCGNCXSSXEF-SFLRWKUSA-N
Formula:	C29H48O
SMILES:	CCC(=CCC(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]:	412.69

Physical Properties

Property code	Value	Unit	Source
gf	291.99	kJ/mol	Joback Method
hf	-421.08	kJ/mol	Joback Method
hfus	40.29	kJ/mol	Joback Method
hvap	94.33	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	7.945		Crippen Method
mvol	373.300	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	4613.00		NIST Webbook
rinpol	4613.00		NIST Webbook
tb	997.18	K	Joback Method
tc	1225.65	K	Joback Method
tf	530.89	K	Joback Method
vc	1.415	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1430.05	J/molxK	997.18	Joback Method
cpg	1463.55	J/molxK	1035.26	Joback Method
cpg	1498.11	J/molxK	1073.34	Joback Method
cpg	1534.10	J/molxK	1111.42	Joback Method
cpg	1571.91	J/molxK	1149.49	Joback Method
cpg	1611.89	J/molxK	1187.57	Joback Method
cpg	1654.44	J/molxK	1225.65	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418789&Units=SI

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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