Stigmasta-7,25-dien-3-ol, (3«beta»,5«alpha»)-

Other names:	5«alpha»-Stigmasta-7,25-dien-3«beta»-ol
	«delta»7,25-Stigmastadienol
	24-Ethyl-5-«alpha»-cholest-7,25-dien-3-«beta»-ol
	24«beta»-Ethyl-5«alpha»-cholesta-7,25-dien-3«beta»-ol
	Stigmasta-7,25(27)-dien-3-ol, (3«beta»,5«alpha»)-
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:	CMQUSRGUOMCHOZ-UHFFFAOYSA-N
Formula:	C29H48O
SMILES:	C=C(C)C(CC)CCC(C)C1CCC2C3=CCC4CC(O)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	412.69
CAS:	6785-58-6

Physical Properties

Property code	Value	Unit	Source
gf	299.61	kJ/mol	Joback Method
hf	-412.87	kJ/mol	Joback Method
hfus	38.81	kJ/mol	Joback Method
hvap	93.70	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	7.945		Crippen Method
mcvol	373.300	ml/mol	McGowan Method
pc	982.69	kPa	Joback Method
rinpol	3325.00		NIST Webbook
tb	989.70	K	Joback Method
tc	1215.93	K	Joback Method
tf	534.21	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1425.71	J/mol×K	989.70	Joback Method
cpg	1458.39	J/mol×K	1027.41	Joback Method
cpg	1491.94	J/mol×K	1065.11	Joback Method

cpg	1526.71	J/mol×K	1102.82	Joback Method
cpg	1563.07	J/mol×K	1140.52	Joback Method
cpg	1601.37	J/mol×K	1178.23	Joback Method
cpg	1641.95	J/mol×K	1215.93	Joback Method

Sources

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=C6785586&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume