Stigmastan-3,5,22-trien

Other names: 24-ethyl-«delta»3,5,22-Cholestatriene
Inchi: InChI=1S/C29H46/c1-7-22(20(2)3)12-11-21(4)25-15-16-26-24-14-13-23-10-8-9-18-28(23
InchiKey: NGUVUCVJXSBIEN-VAWYXSNFSA-N
Formula: C29H46
SMILES: CCC(C=CC(C)C1CCC2C3CC=C4C=CCCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 394.68

Physical Properties

Property code	Value	Unit	Source
gf	472.59	kJ/mol	Joback Method
hf	-186.22	kJ/mol	Joback Method
hfus	34.14	kJ/mol	Joback Method
hvap	77.78	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	8.606		Crippen Method
mcvol	363.130	ml/mol	McGowan Method
pc	976.56	kPa	Joback Method
rinpol	2990.00		NIST Webbook
rinpol	2981.00		NIST Webbook
rinpol	2990.00		NIST Webbook
rinpol	2981.00		NIST Webbook
tb	908.51	K	Joback Method
tc	1138.78	K	Joback Method
tf	474.03	K	Joback Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1300.72	J/mol×K	908.51	Joback Method
cpg	1332.33	J/mol×K	946.89	Joback Method
cpg	1364.26	J/mol×K	985.27	Joback Method
cpg	1396.90	J/mol×K	1023.65	Joback Method
cpg	1430.65	J/mol×K	1062.03	Joback Method

cpg	1465.90	J/mol×K	1100.40	Joback Method
cpg	1503.03	J/mol×K	1138.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U214181&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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