24-Ethylcholesta-5,7-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: ARVGMISWLZPBCH-GODUPTBPSA-N
Formula: C29H48O
SMILES: CCC(CCC(C)C1CCC2C3=CC=C4CC(O)CCC4(C)C3CCC21C)C(C)C
Mol. weight [g/mol]: 412.69

Physical Properties

Property code	Value	Unit	Source
gf	245.92	kJ/mol	Joback Method
hf	-467.14	kJ/mol	Joback Method
hfus	37.64	kJ/mol	Joback Method
hvap	95.16	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	7.945		Crippen Method
mcvol	373.300	ml/mol	McGowan Method
pc	992.00	kPa	Joback Method
rinpol	3285.00		NIST Webbook
rinpol	3335.00		NIST Webbook
tb	1001.51	K	Joback Method
tc	1229.27	K	Joback Method
tf	552.45	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1424.19	J/mol×K	1001.51	Joback Method
cpg	1457.07	J/mol×K	1039.47	Joback Method
cpg	1490.99	J/mol×K	1077.43	Joback Method
cpg	1526.29	J/mol×K	1115.39	Joback Method
cpg	1563.32	J/mol×K	1153.35	Joback Method
cpg	1602.45	J/mol×K	1191.31	Joback Method
cpg	1644.04	J/mol×K	1229.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R214285&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
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
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