24-Ethylcholesta-5,7,22-trien-3-«beta»-ol

Inchi: InChI=1S/C29H46O/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: OQMZNAMGEHIHNN-KNDDKGQDSA-N
Formula: C29H46O
SMILES: CCC(C=CC(C)C1CCC2C3=CC=C4CC(O)CCC4(C)C3CCC21C)C(C)C
Mol. weight [g/mol]: 410.67

Physical Properties

Property code	Value	Unit	Source
gf	326.14	kJ/mol	Joback Method
hf	-349.92	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	95.12	kJ/mol	Joback Method
log10ws	-8.54		Crippen Method
logp	7.721		Crippen Method
mcvol	369.000	ml/mol	McGowan Method
pc	1025.31	kPa	Joback Method
rinpol	3280.00		NIST Webbook
tb	1005.67	K	Joback Method
tc	1236.26	K	Joback Method
tf	547.37	K	Joback Method
vc	1.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1397.14	J/mol×K	1005.67	Joback Method
cpg	1430.45	J/mol×K	1044.10	Joback Method
cpg	1465.04	J/mol×K	1082.53	Joback Method
cpg	1501.31	J/mol×K	1120.97	Joback Method
cpg	1539.64	J/mol×K	1159.40	Joback Method
cpg	1580.41	J/mol×K	1197.83	Joback Method
cpg	1624.02	J/mol×K	1236.26	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=R490434&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